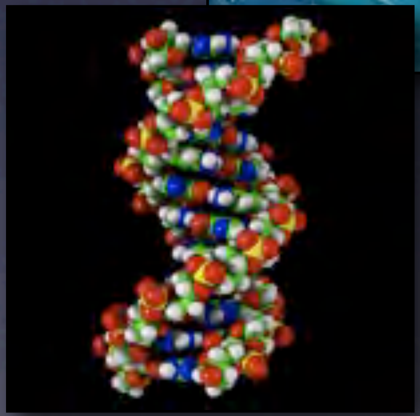
Neutron Acceptance Diagram Shading

Phil Bentley
ILL

Why?

- New problems in optics often involve optimisation in many-dimensional parameter spaces
- May have lots of local optima
- Analytical solutions might not exist

- Nature has solved such optimisation problems already

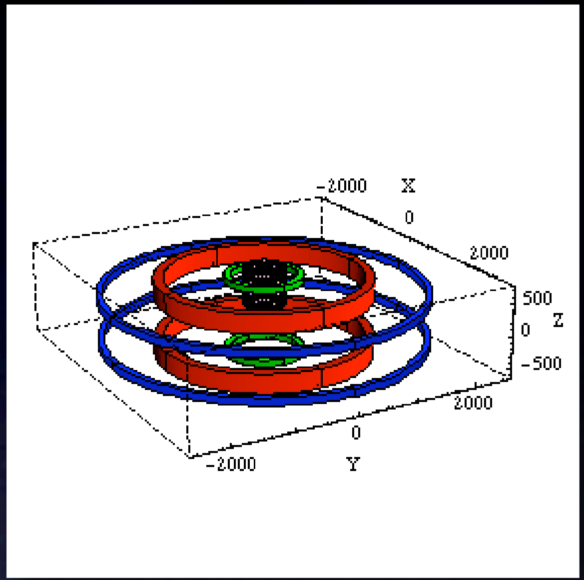


Why?

- Particle swarms / genetic algorithms need 100 iterations or more to converge
- Each iteration evaluates 30-50 agents
- Therefore, 3000 simulations minimum
- Either use a cluster or something other than Monte-Carlo

A.I. Works Well

- Complex geometry with many coupled parameters



- SPAN-cryopad
- multi-channel guides IN5
- WASP
- TYREX ^{3}He polariser (new model)

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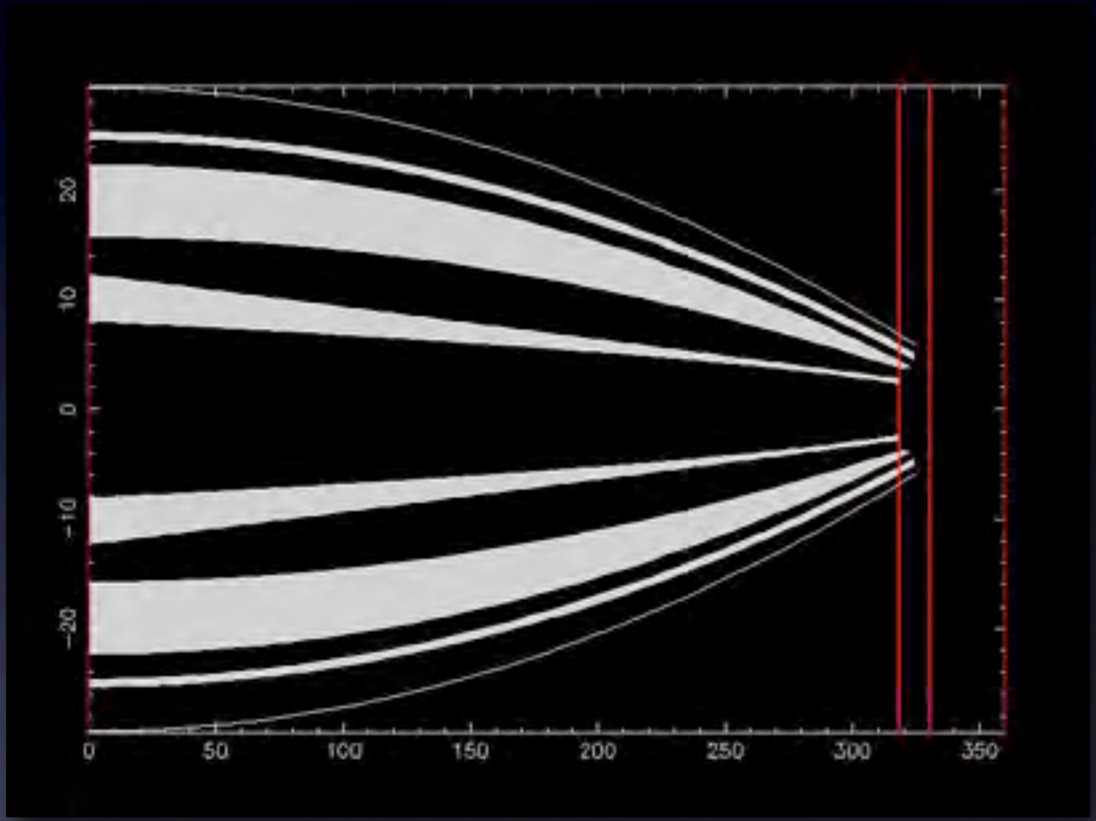

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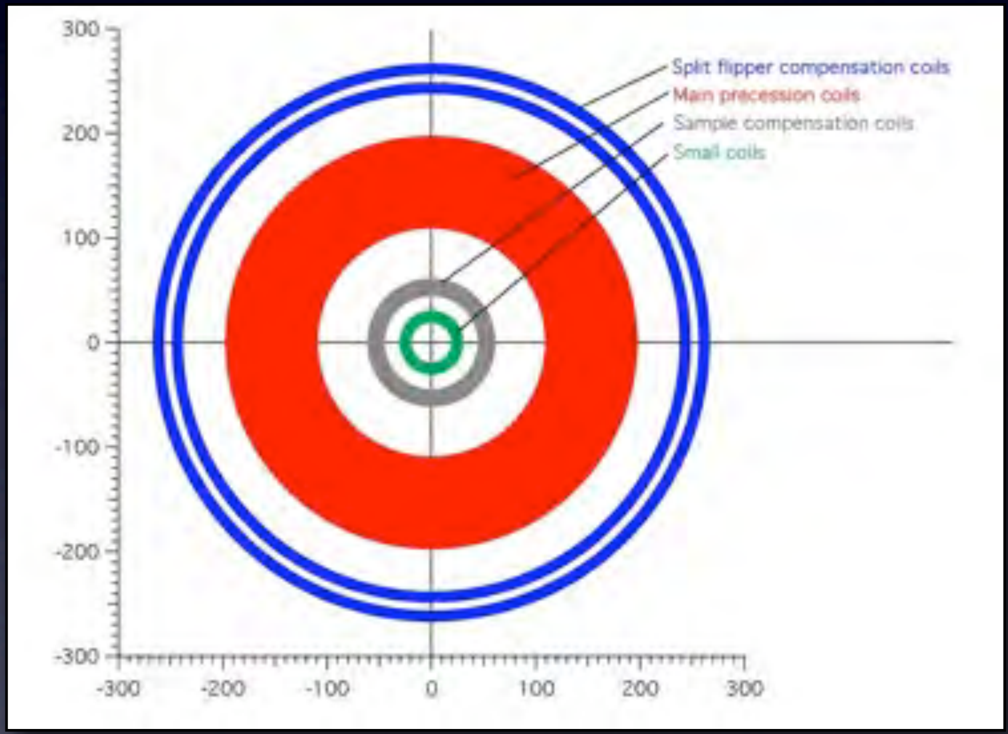

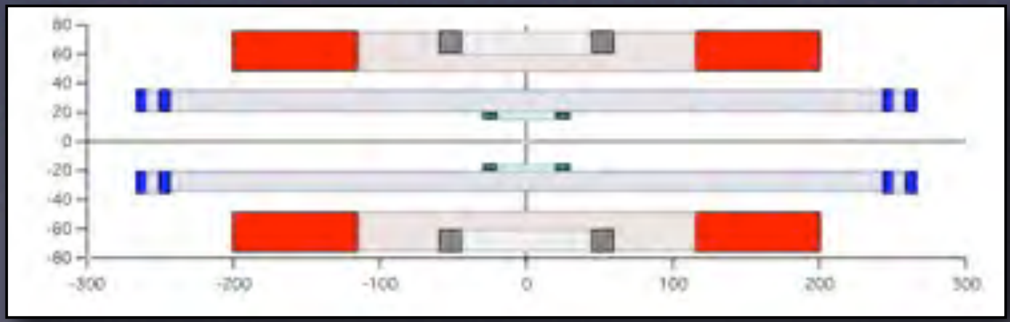

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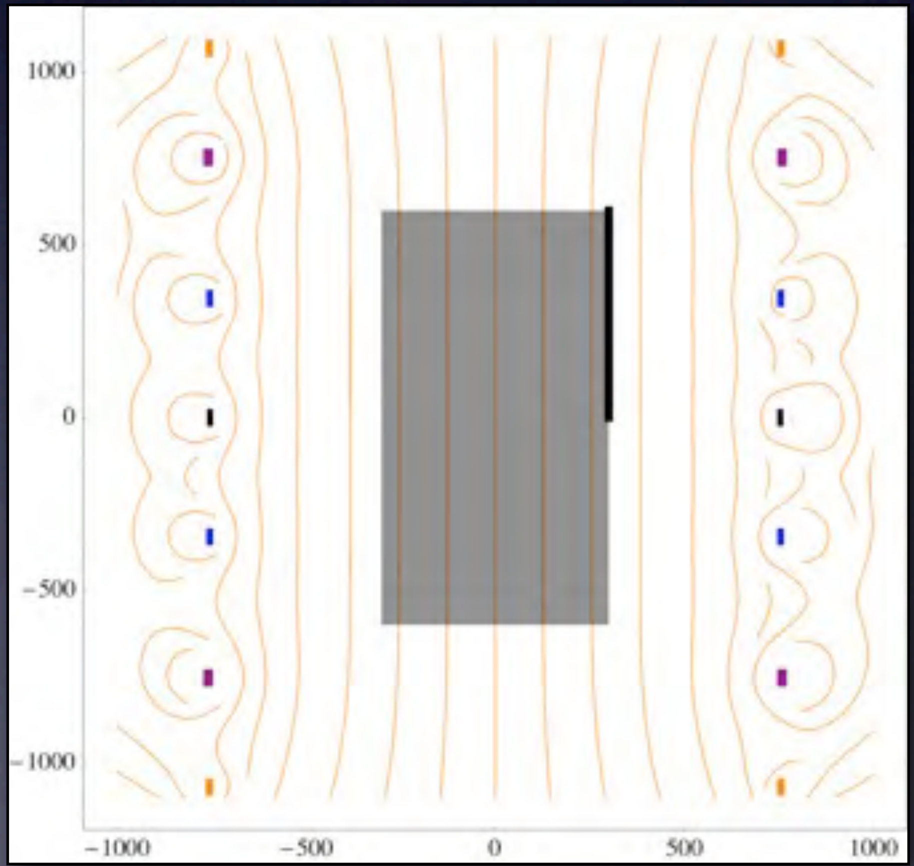
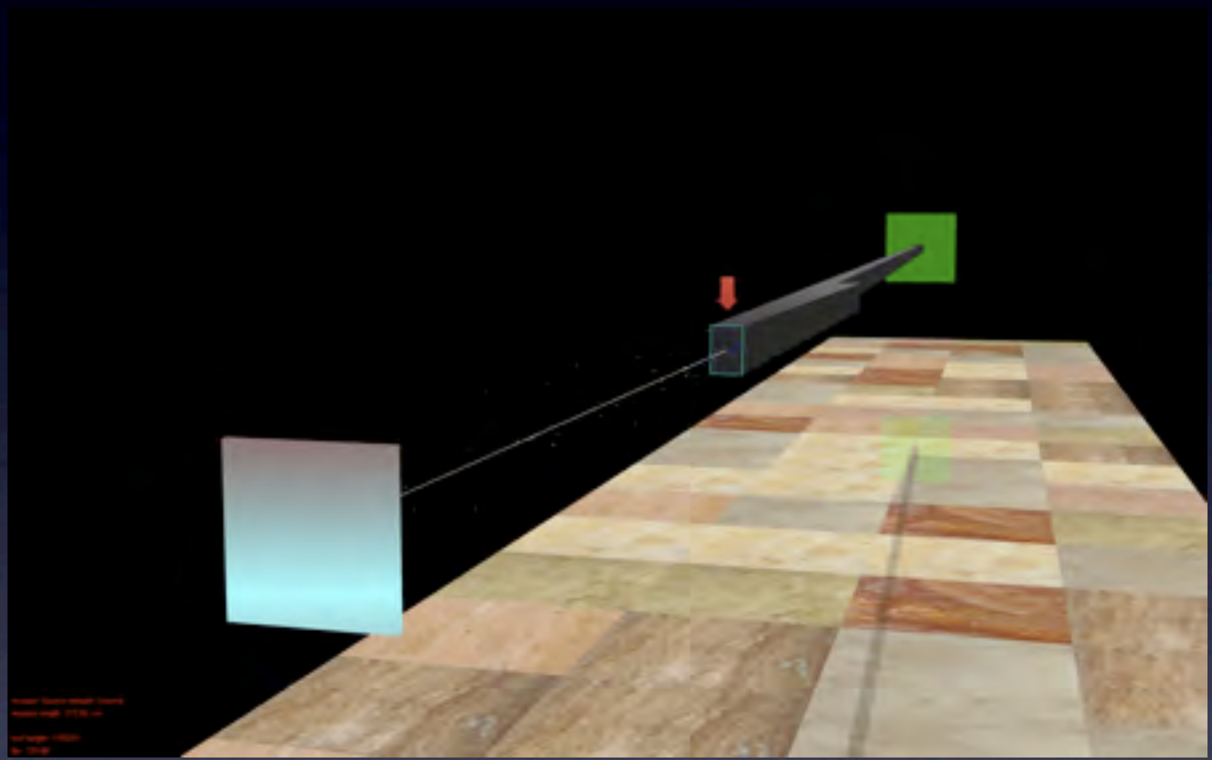


Full Optimisations

- Simulate the instrument all the way from moderator to detector
- All parameters free
- Don't care if parameters are strongly coupled
- Parameter limit: >47 but <650 with canonical algorithms



SANS on D22

- 100 000 000 trajectories *entering the guide*
- 666 seconds CPU time (11 minutes) => 74 trajectories hit the sample
- Statistical error = 12%
- 1% error needs 25 hours
- Optimisation of D22: 8-25 *years* (1 cpu)

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nads Speed Gain

http://flickr.com/photos/17393884@N00/5341048/ Flickr

→

1.5 x

http://www.apolloarchive.com/apollo_gallery.html

Similar Problem Solved

- Ray tracing is routinely used in movies
- Very slow! Scenes rendered on huge clusters
- Vector graphics is close to ray trace quality
- 30 frames per second

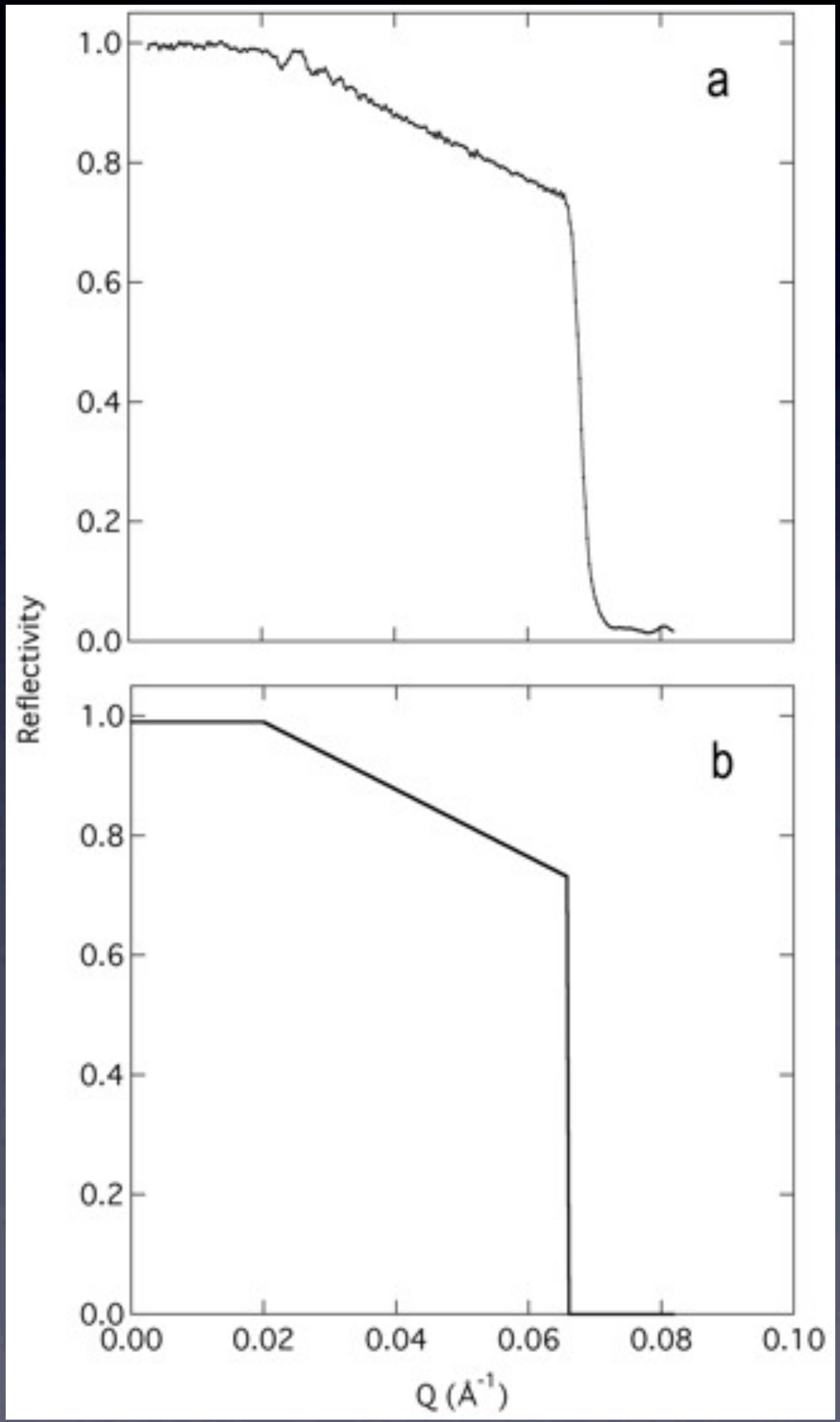
Similar Problem Solved

Neutron Bunches

- The analogy is to group trajectories into "similar" bunches and treat the group as one single object.
- Bunches are phase space regions with linear relation between trajectories
- How do we separate the bunches so the calculation remains accurate?

Guide Reflectivity

- Divide bunches along m=1 and critical m.
- Trajectories within a bunch are linearly dependent
- Guide reflectivity is an idealised curve
- R at m_crit taken from Swiss neutronics

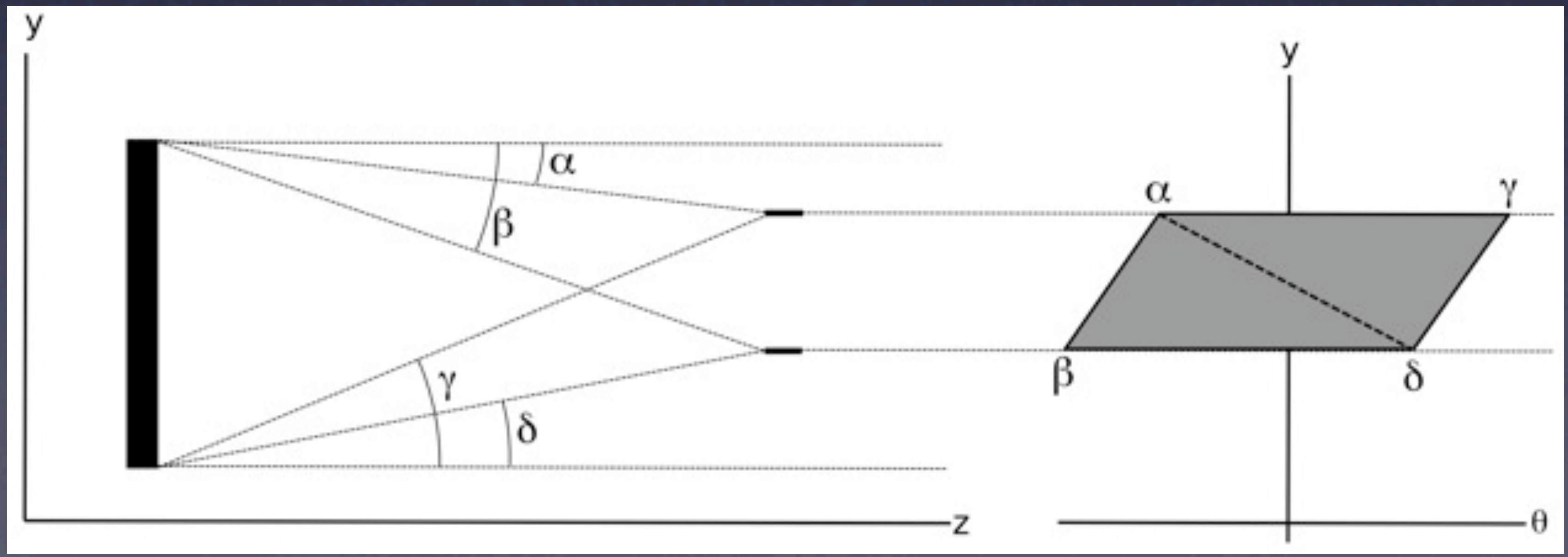


Acceptance Diagrams

- Define boundaries in distance-divergence space
- Division is on module-by-module basis

Source Module

- Just like Monte-Carlo, we have a source plane and a virtual “exit window”.
- Exit window must be at least as large as subsequent module
- Propagation = shear



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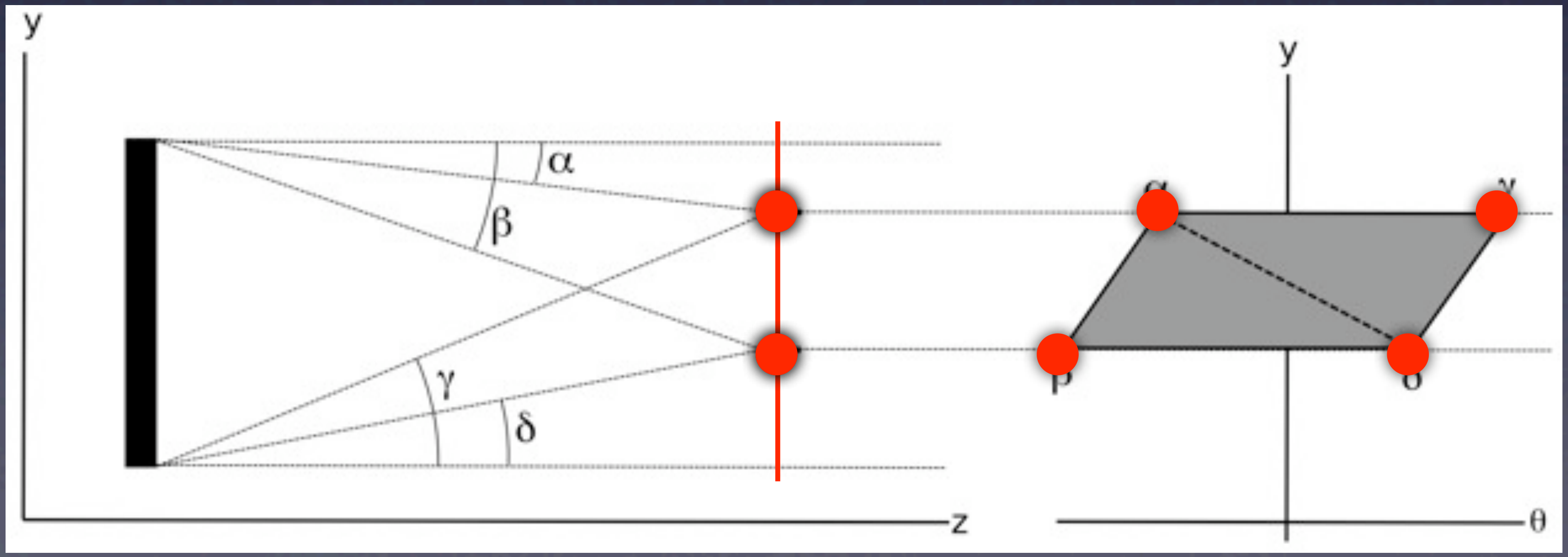

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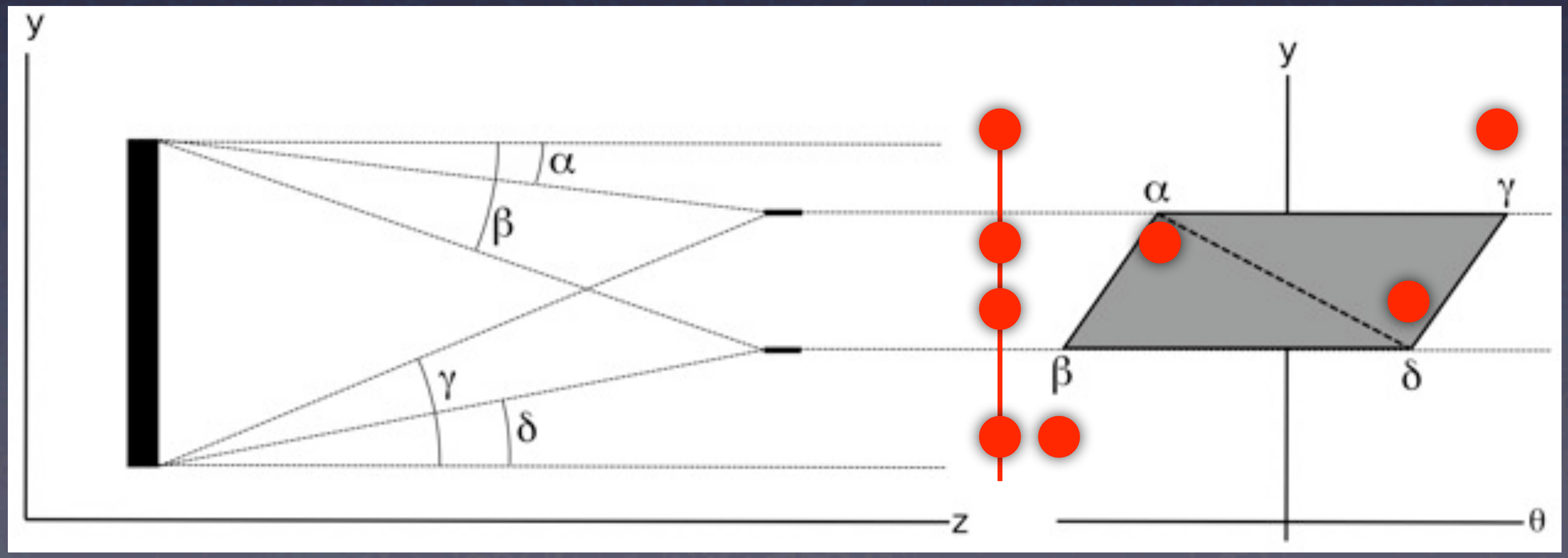
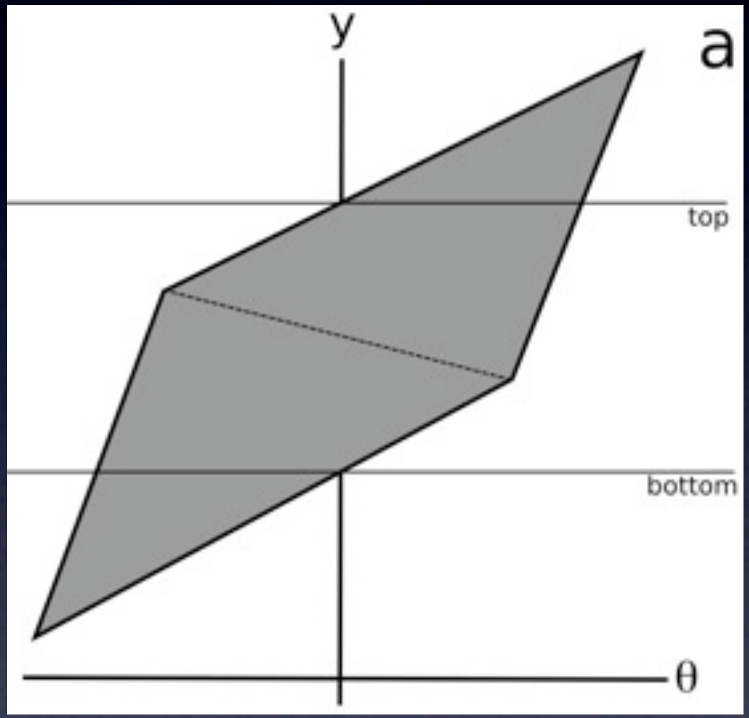


Collimator/Aperture

- For aperture clip off extrema in space axis
- For collimator, clip off extrema in divergence axis



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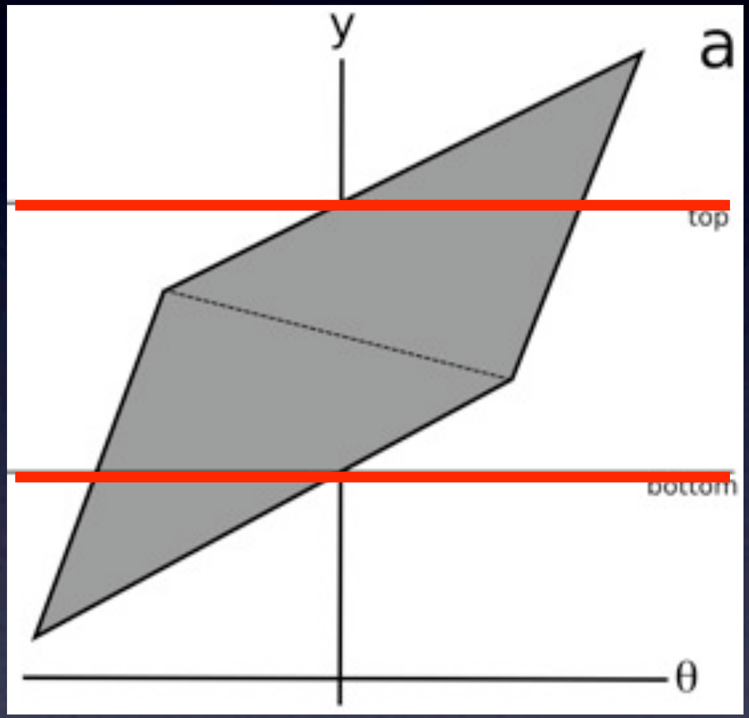

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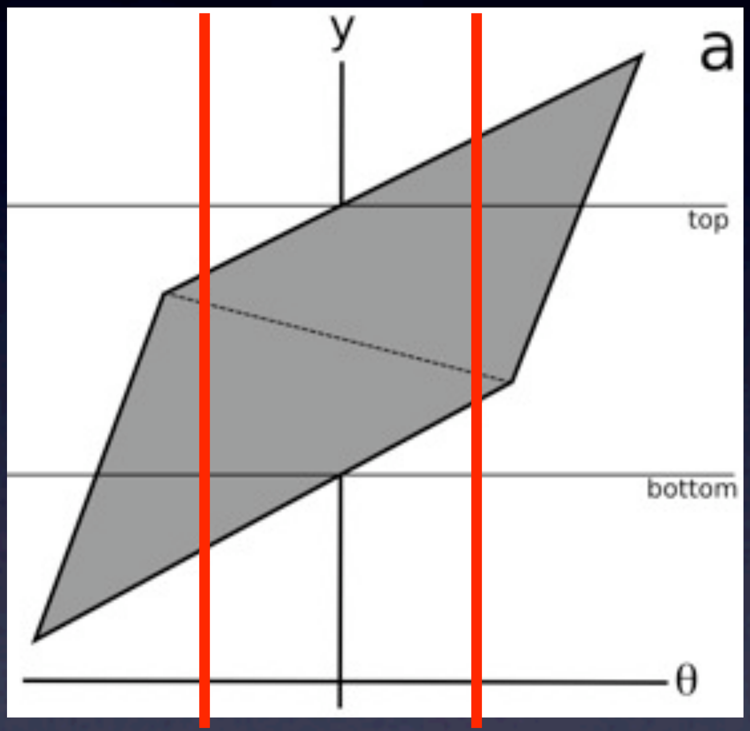
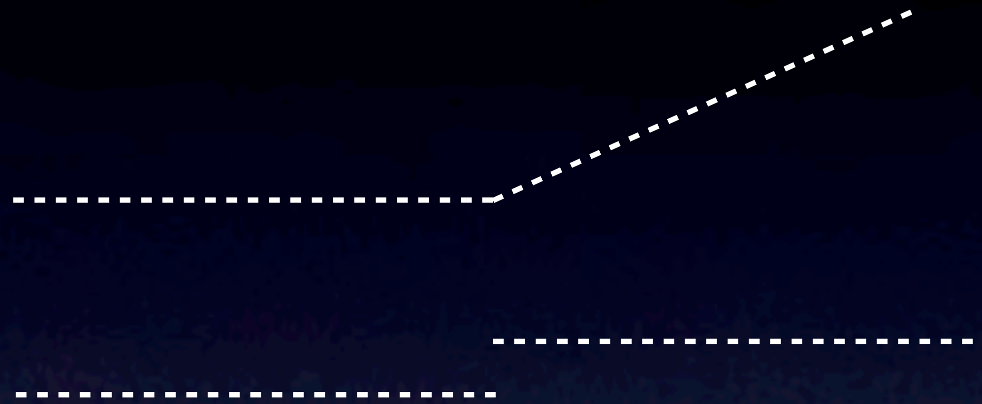
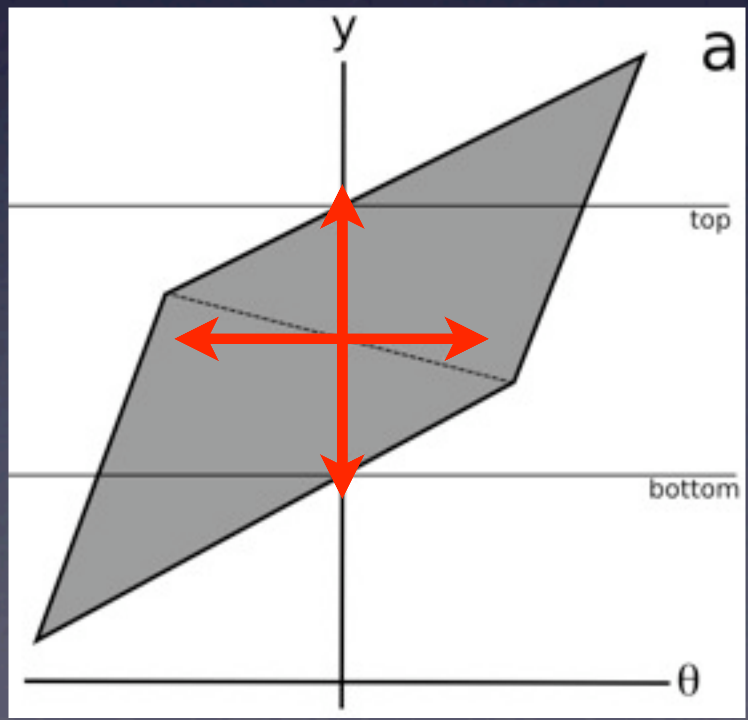


Change Coordinates

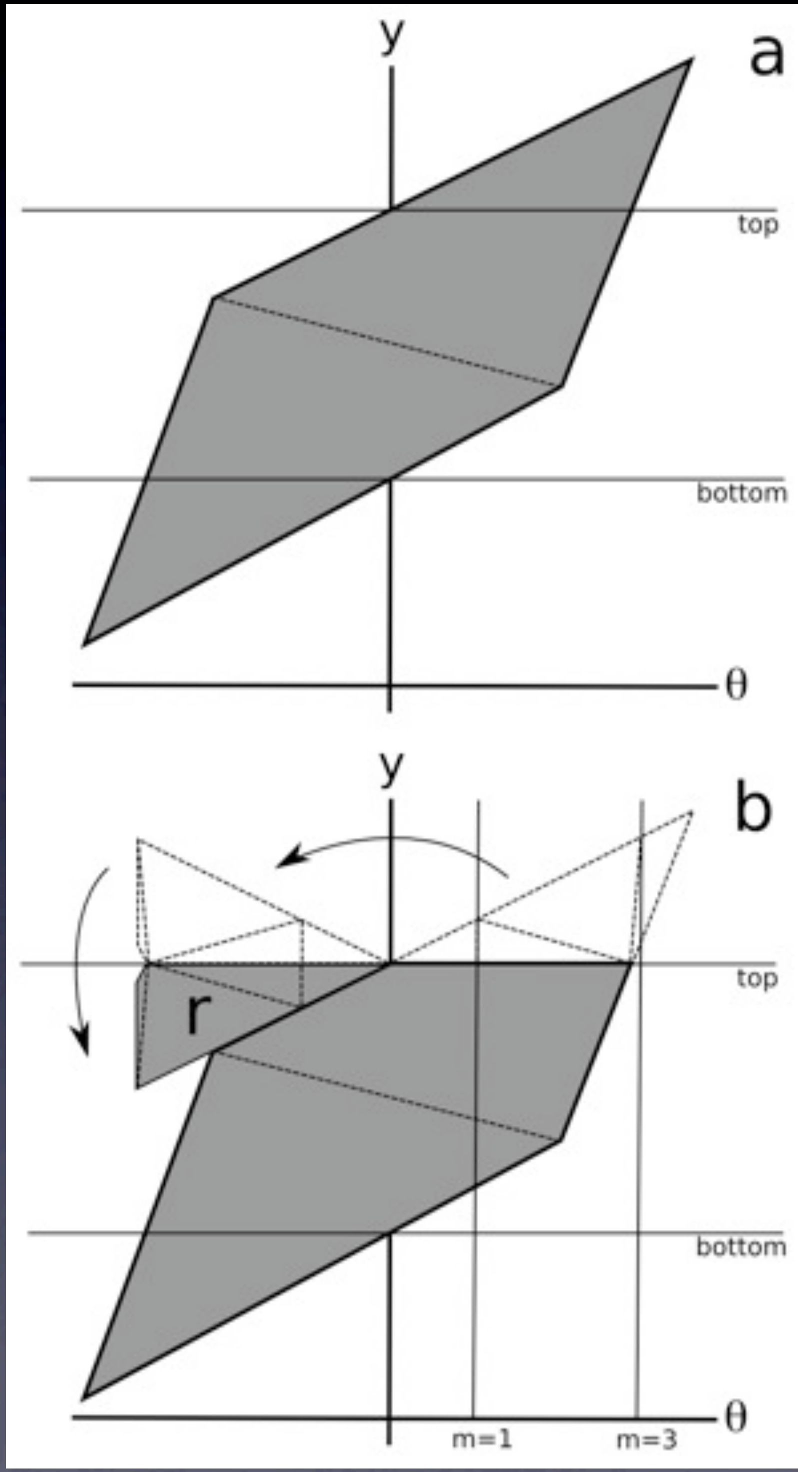


- Rotate beam axis
- Translate beam axis
- Both are a translation of phase space volumes



Guide Module

- Kill neutrons that miss the entrance
- Propagate neutrons to the end of the guide
- Divide along m boundaries
- Multiply reflected weight by reflectivity



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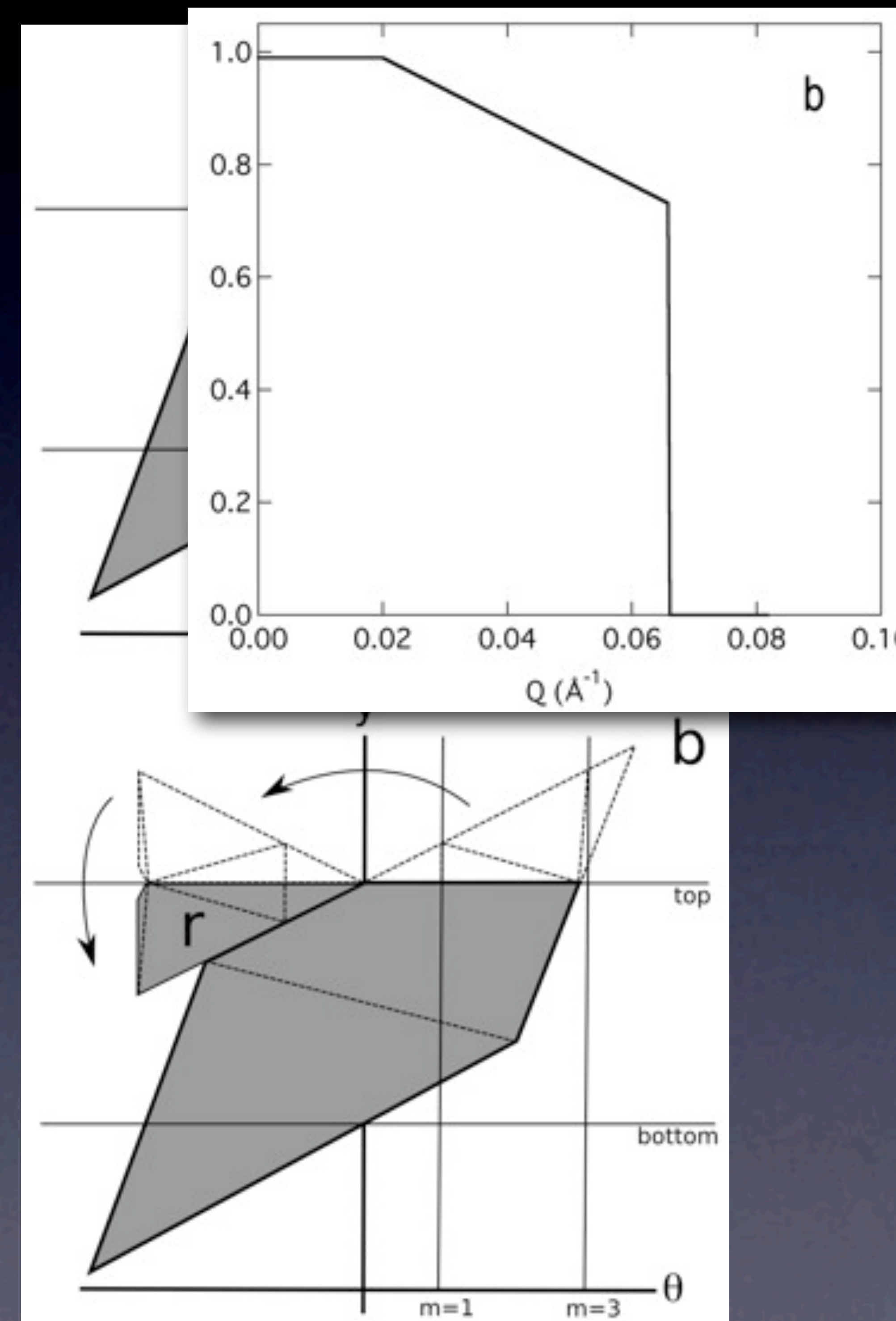

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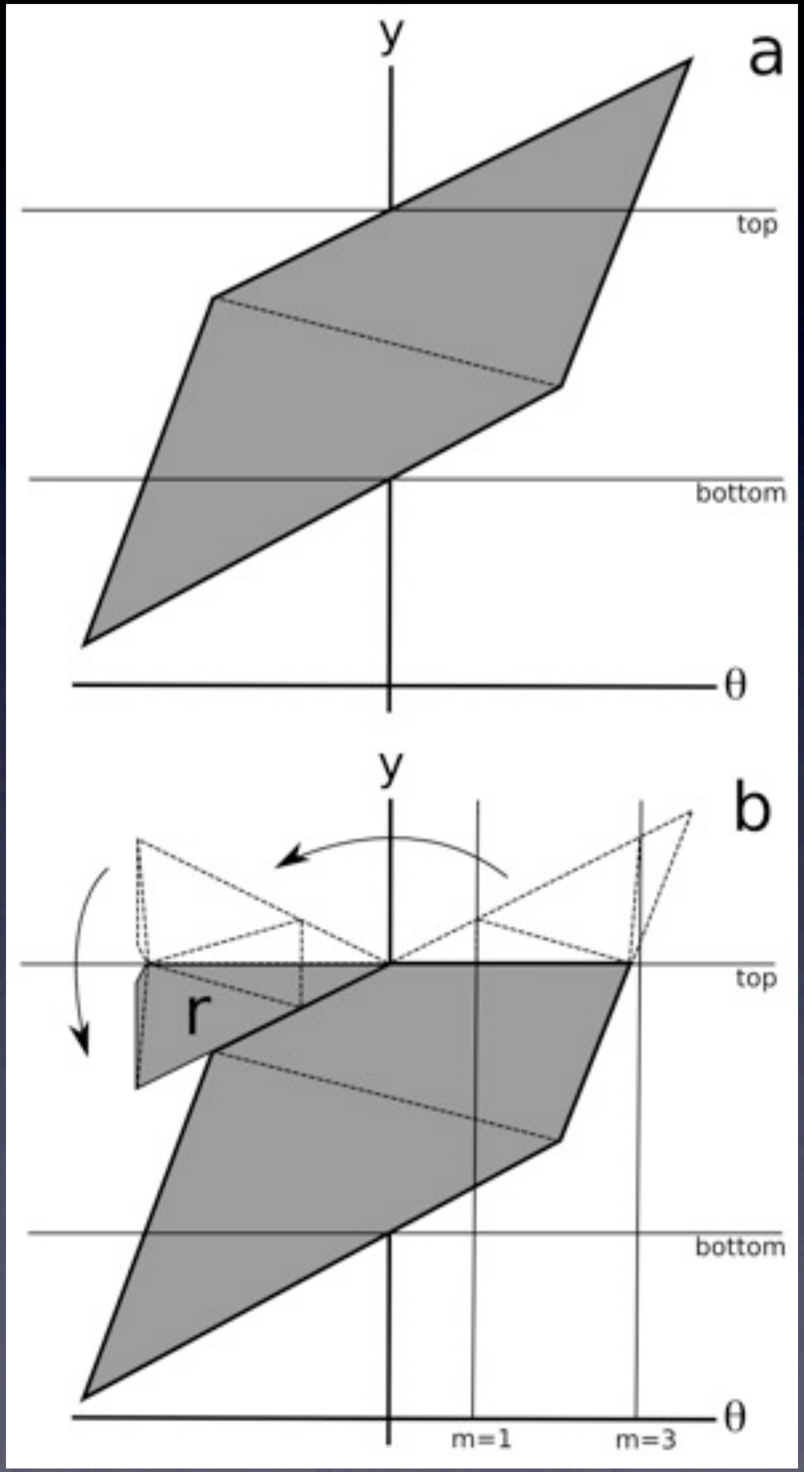
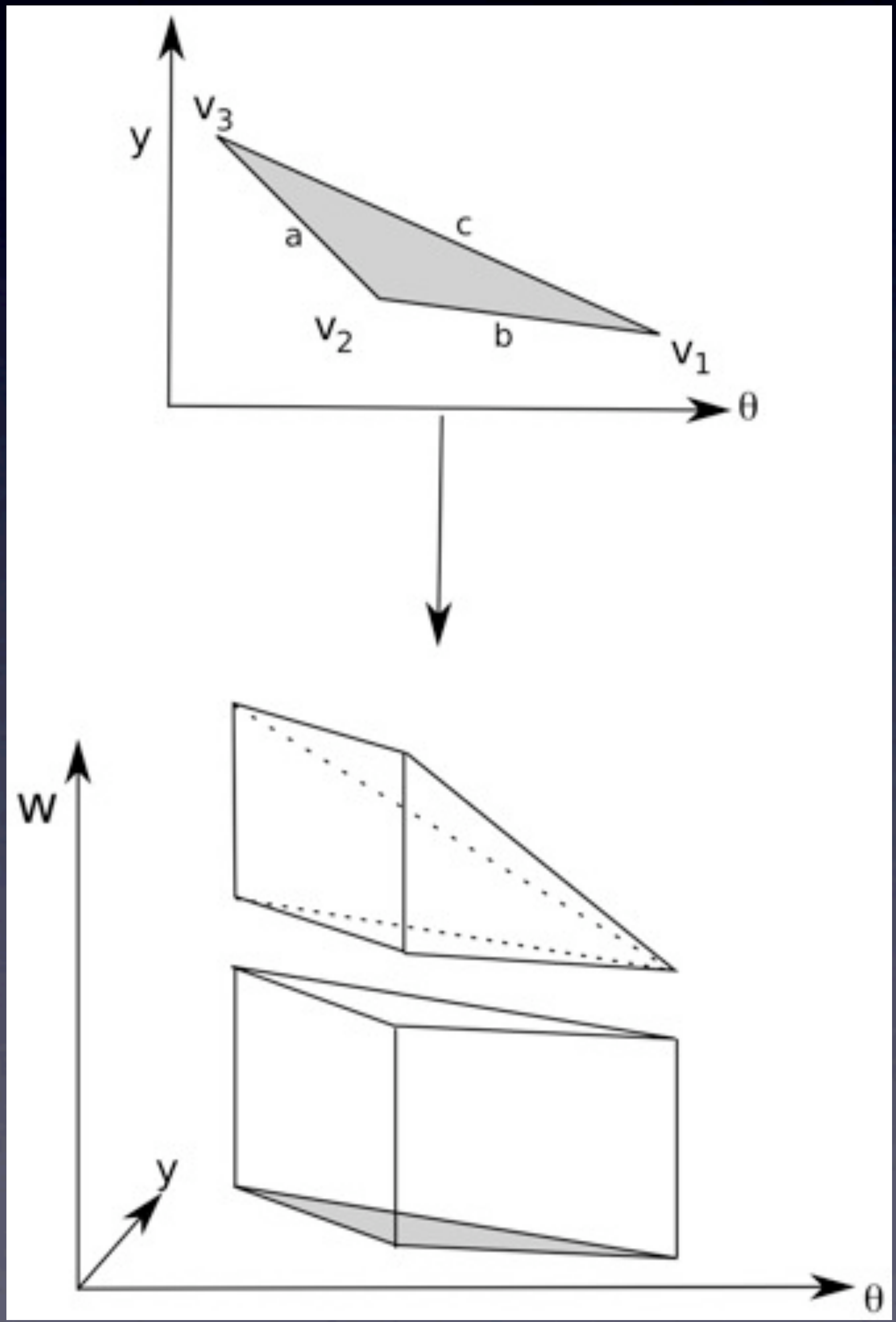


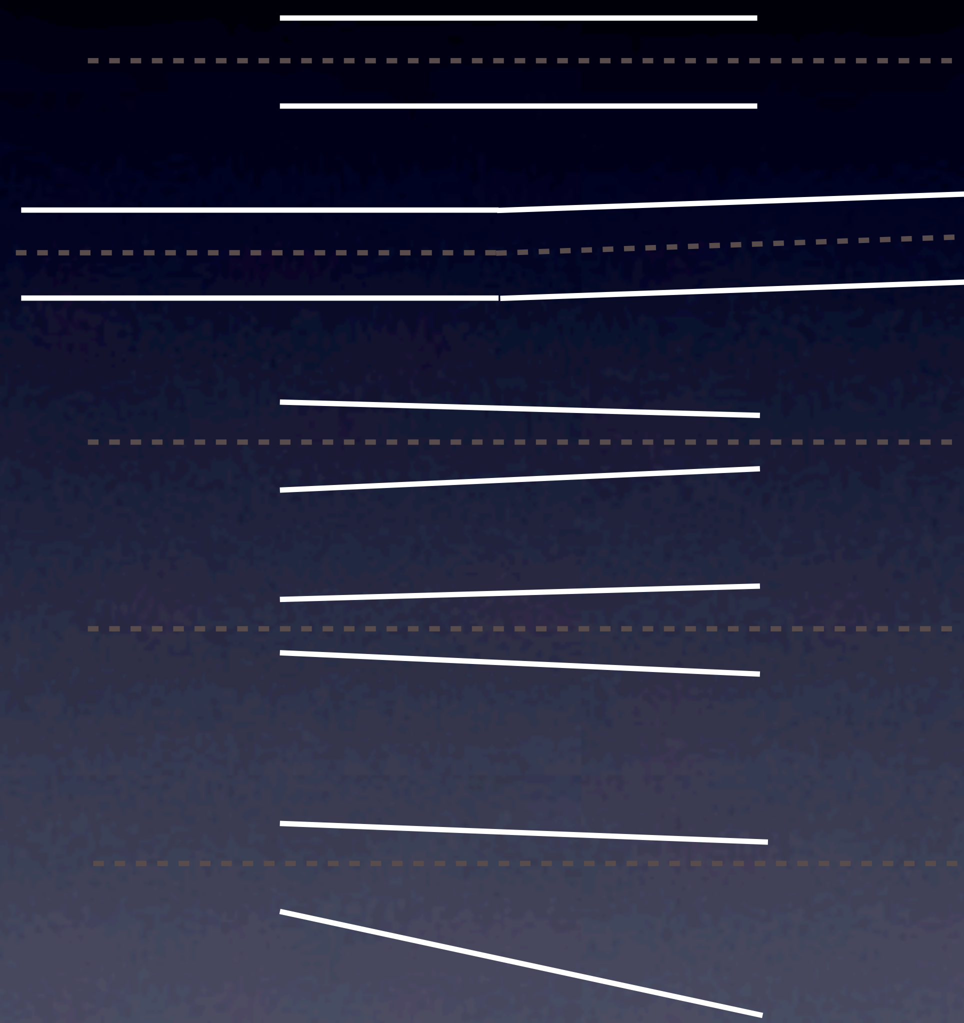
Statistical Weight

- Use triangular primitives
- Statistical weight of a triangle is a volume calculation
- Right-wedge plus square-based pyramid
- Only difficulty is very thin triangles (known problem in CS)

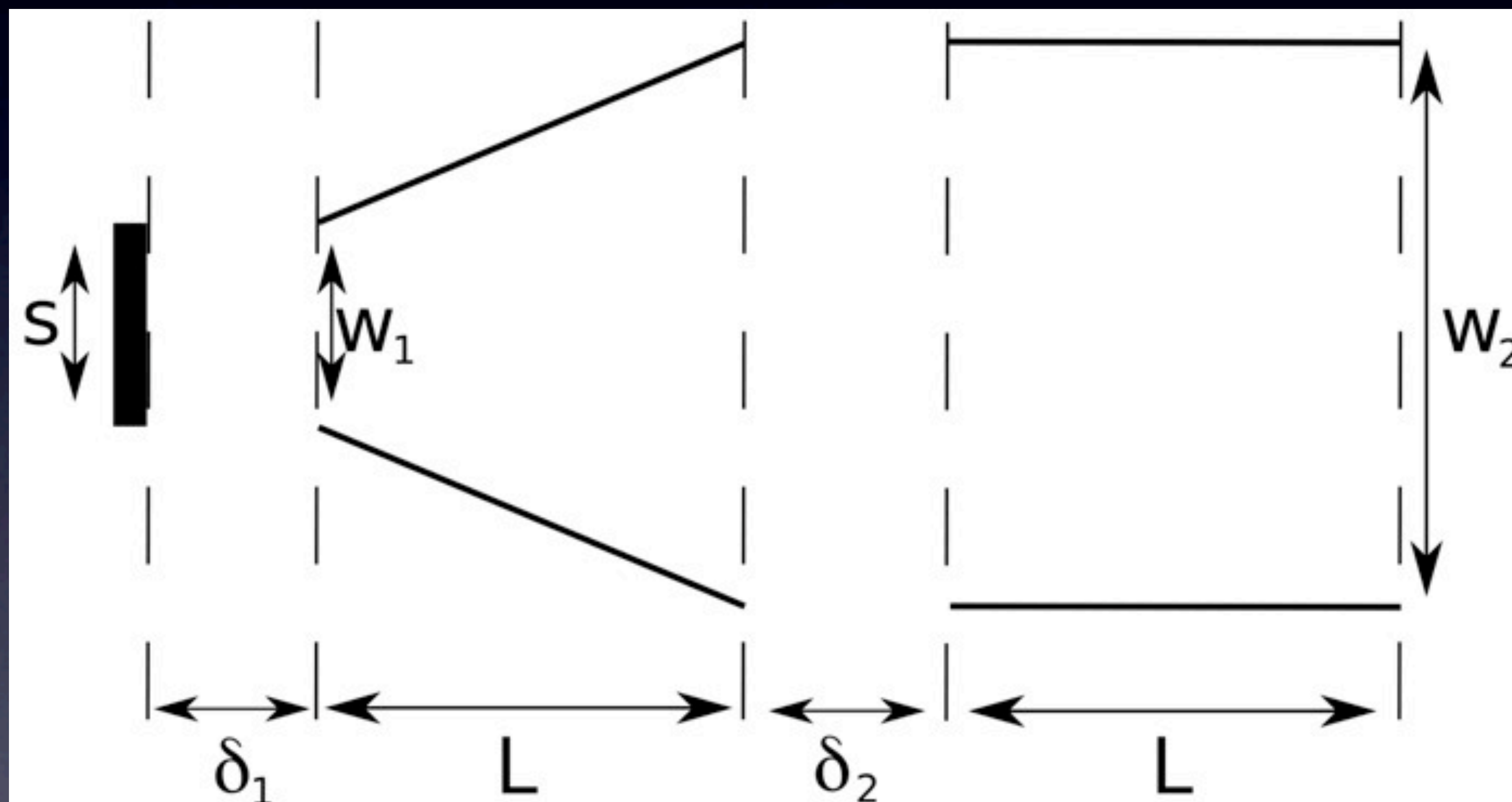


Guides Supported

- Straight
- Curved parallel
- Converging
- Diverging
- Arbitrary



Test 1: Simple Guide



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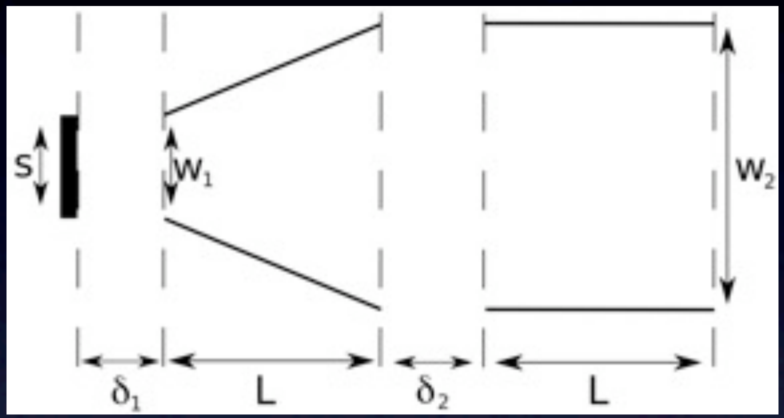

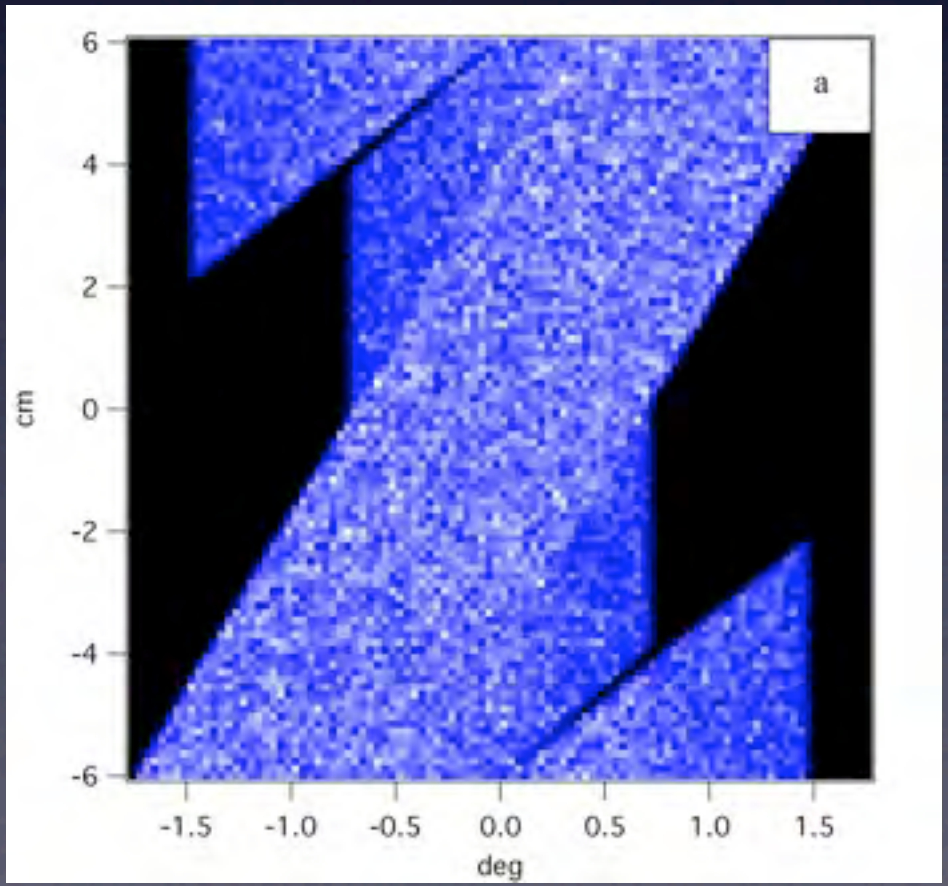

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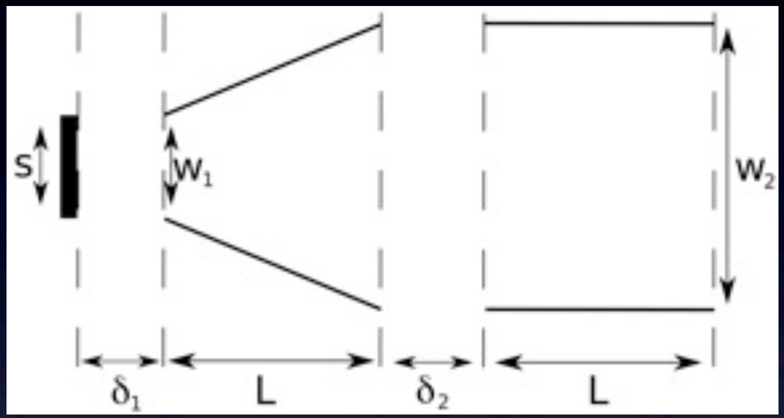

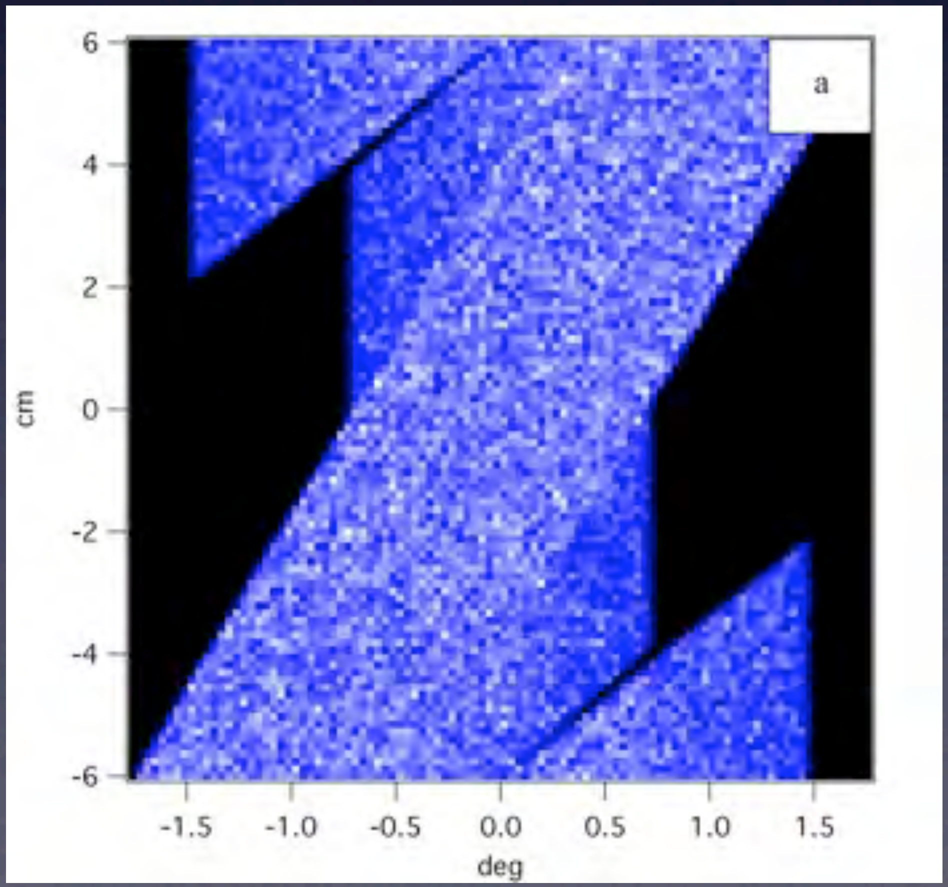

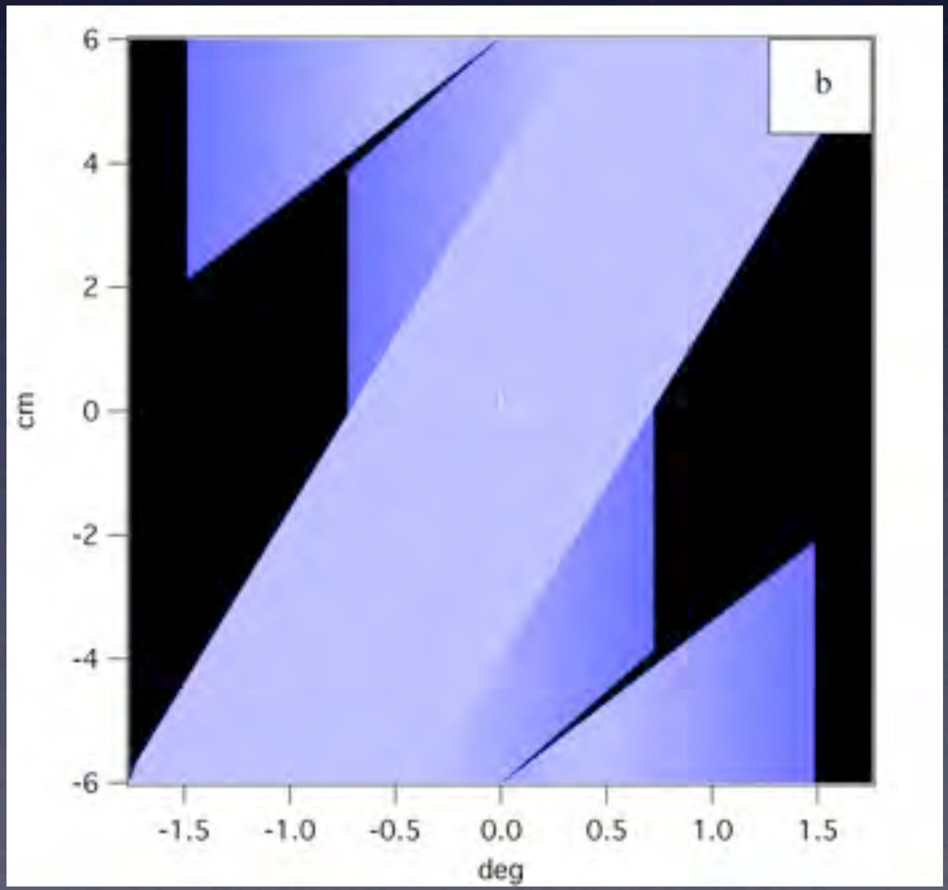

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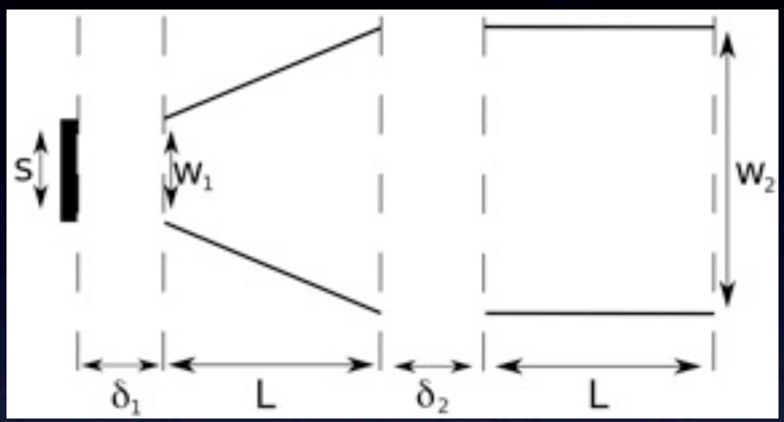

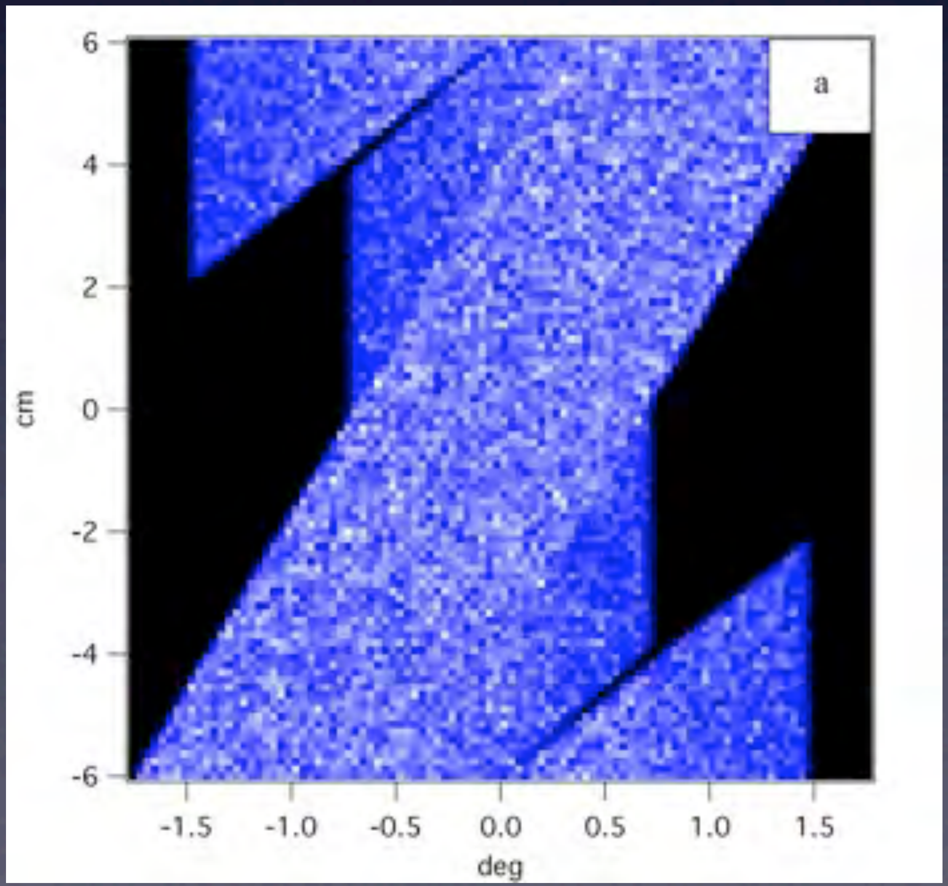

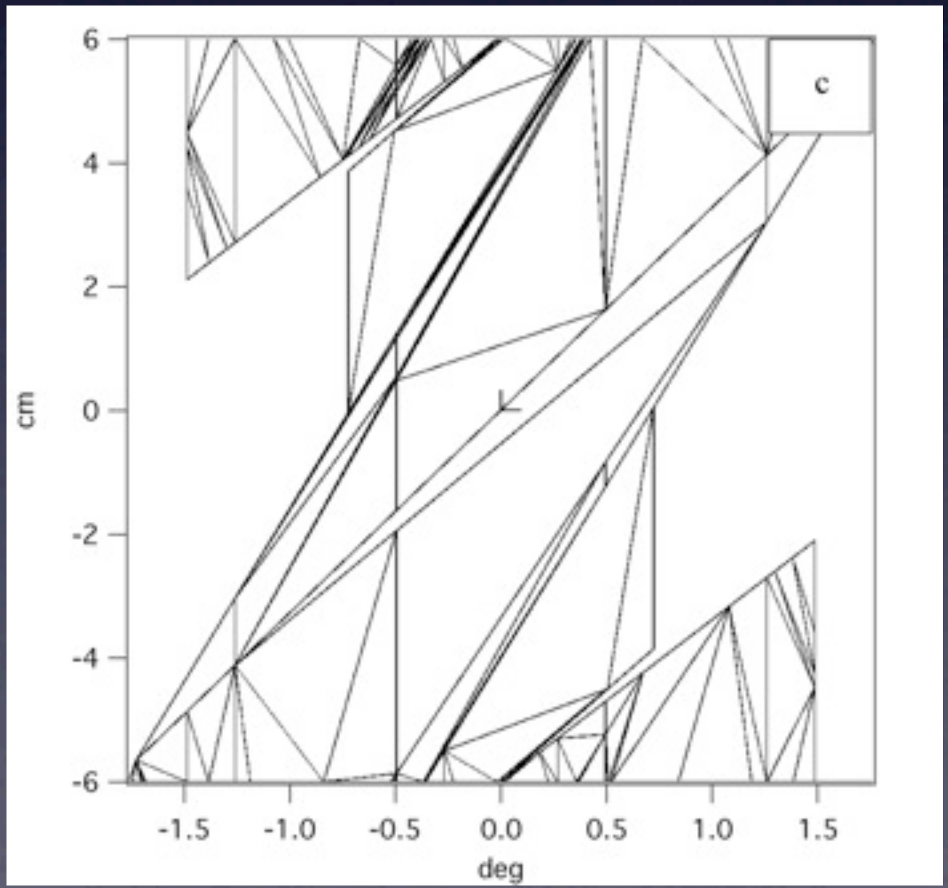

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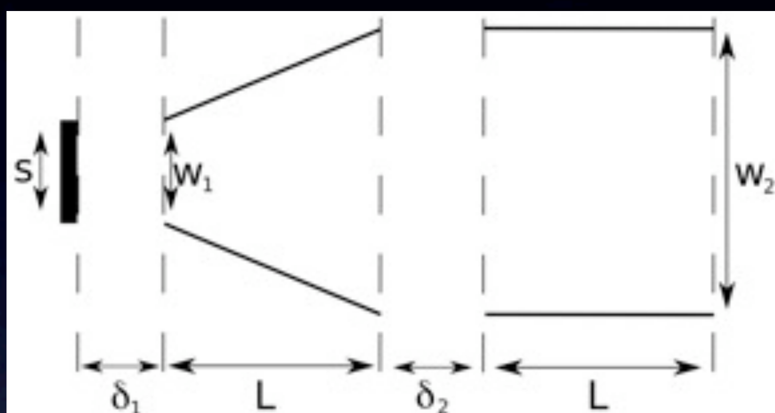
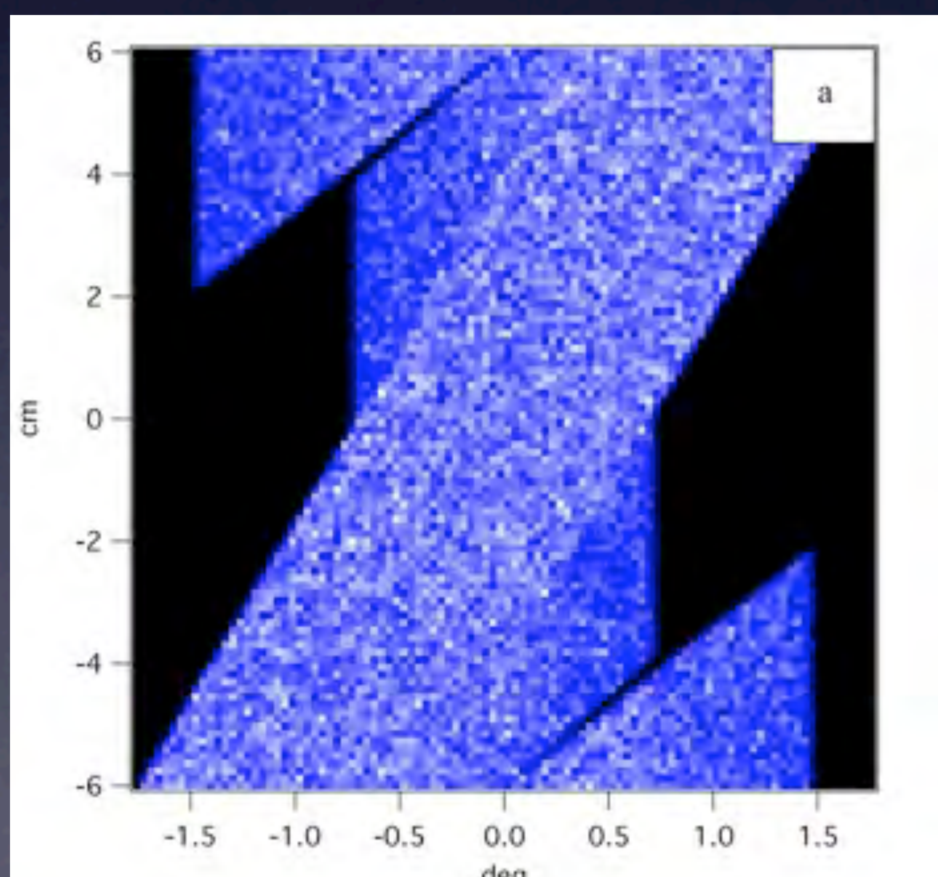
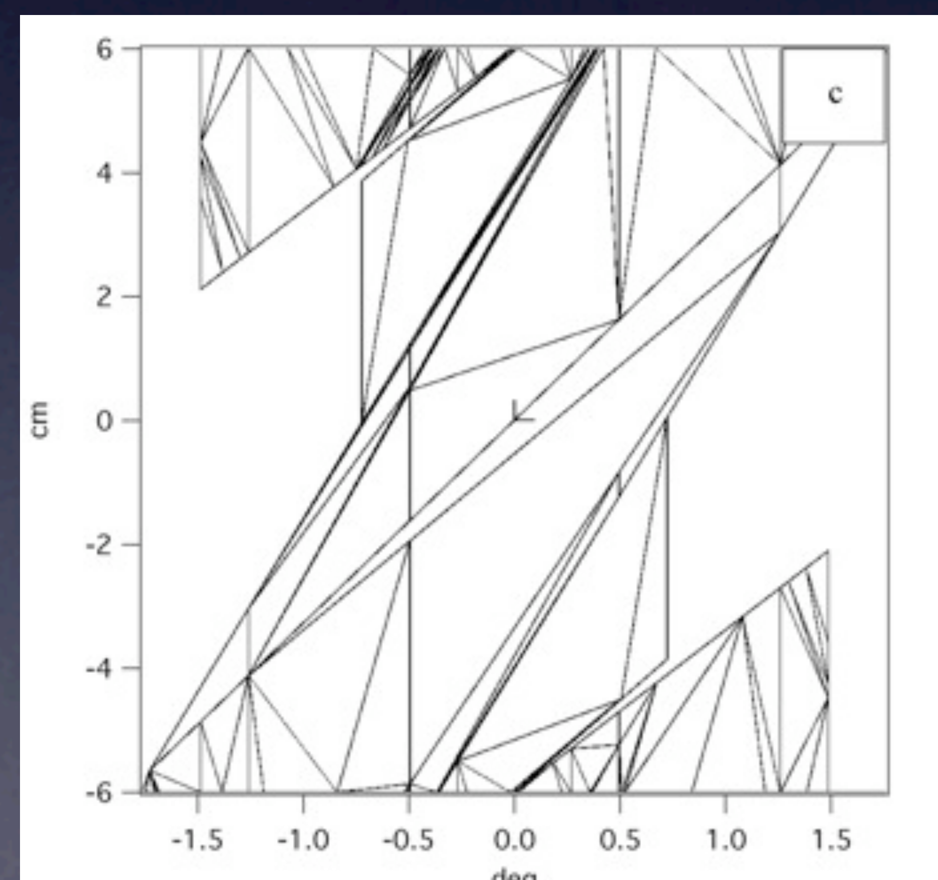




2% Error, 4.8 s



48 ms

Test 2: D22 (V)

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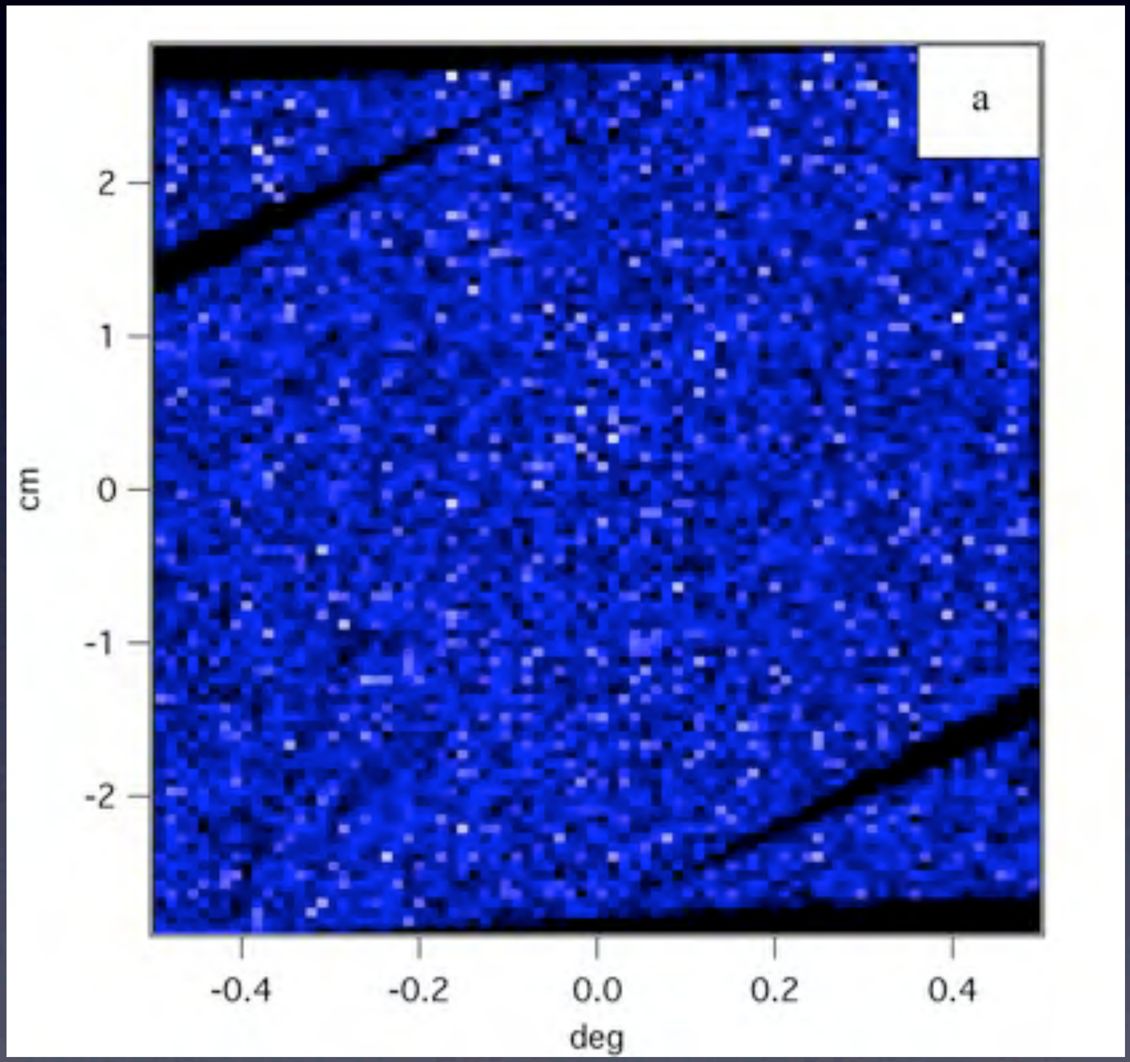

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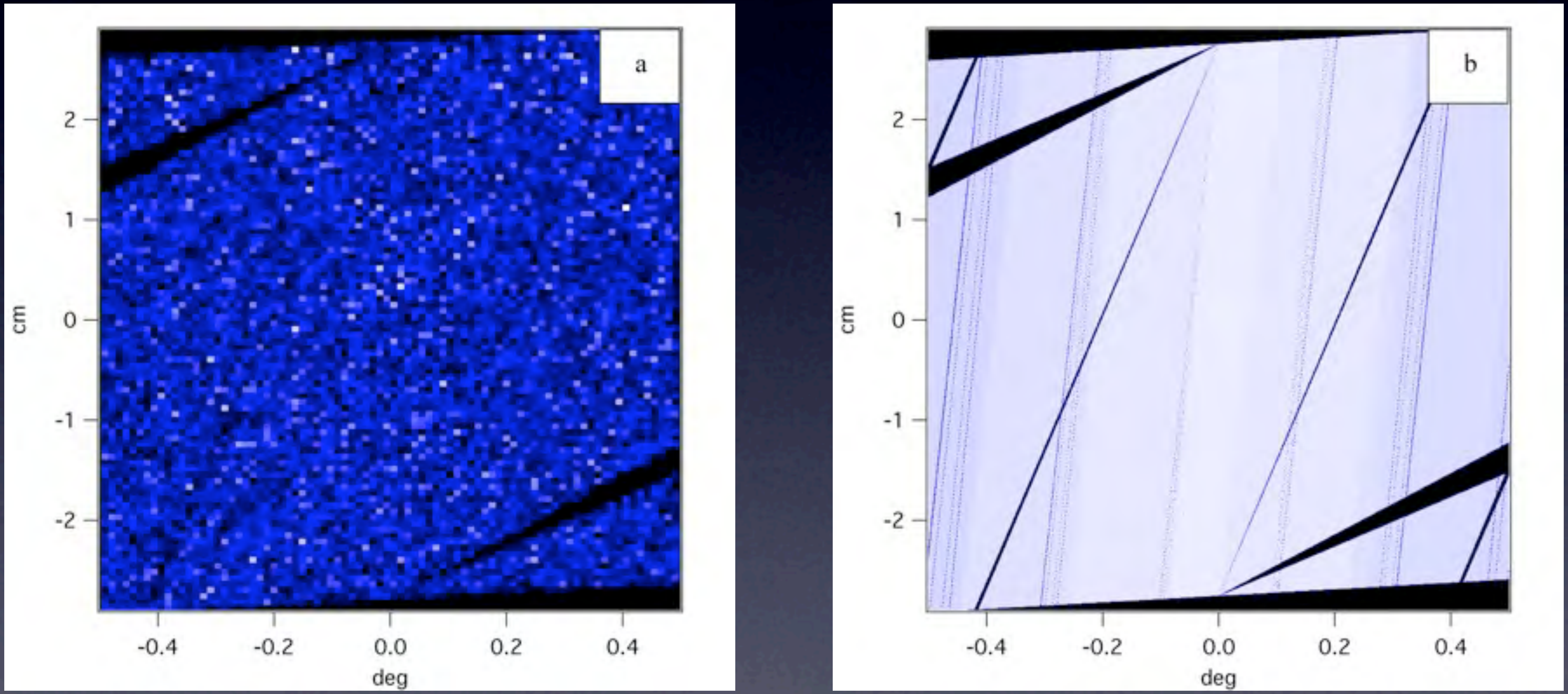

Test 2: D22 (H)

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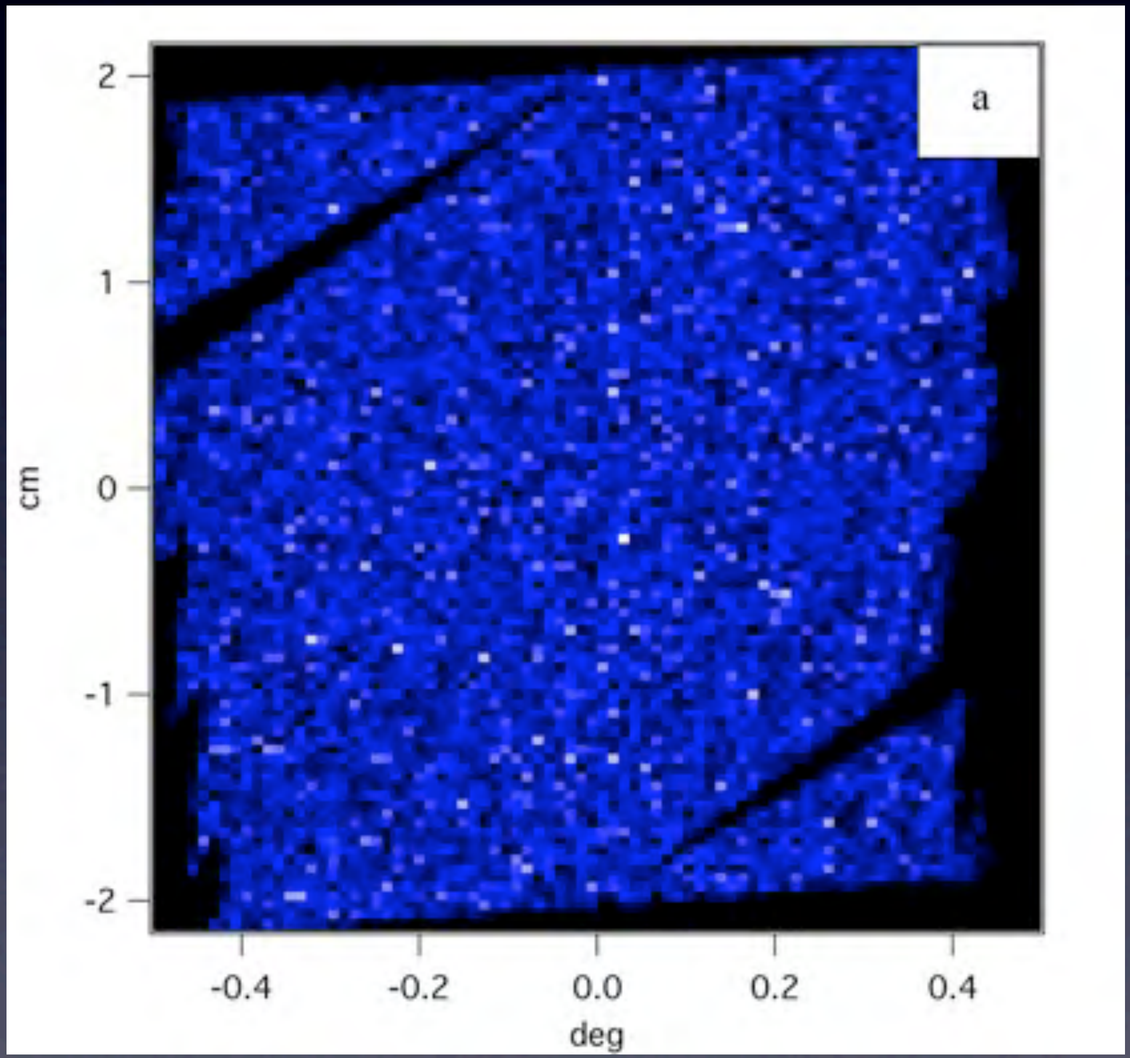

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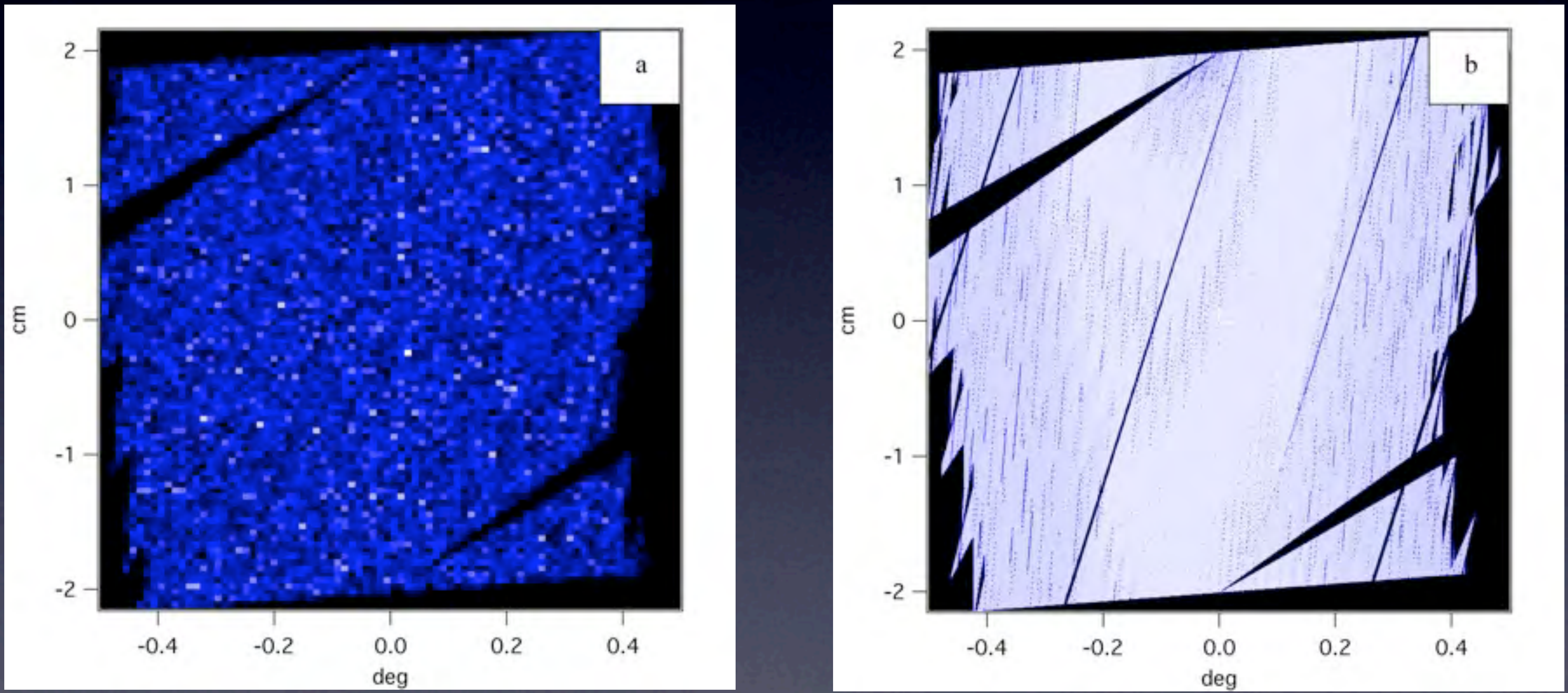

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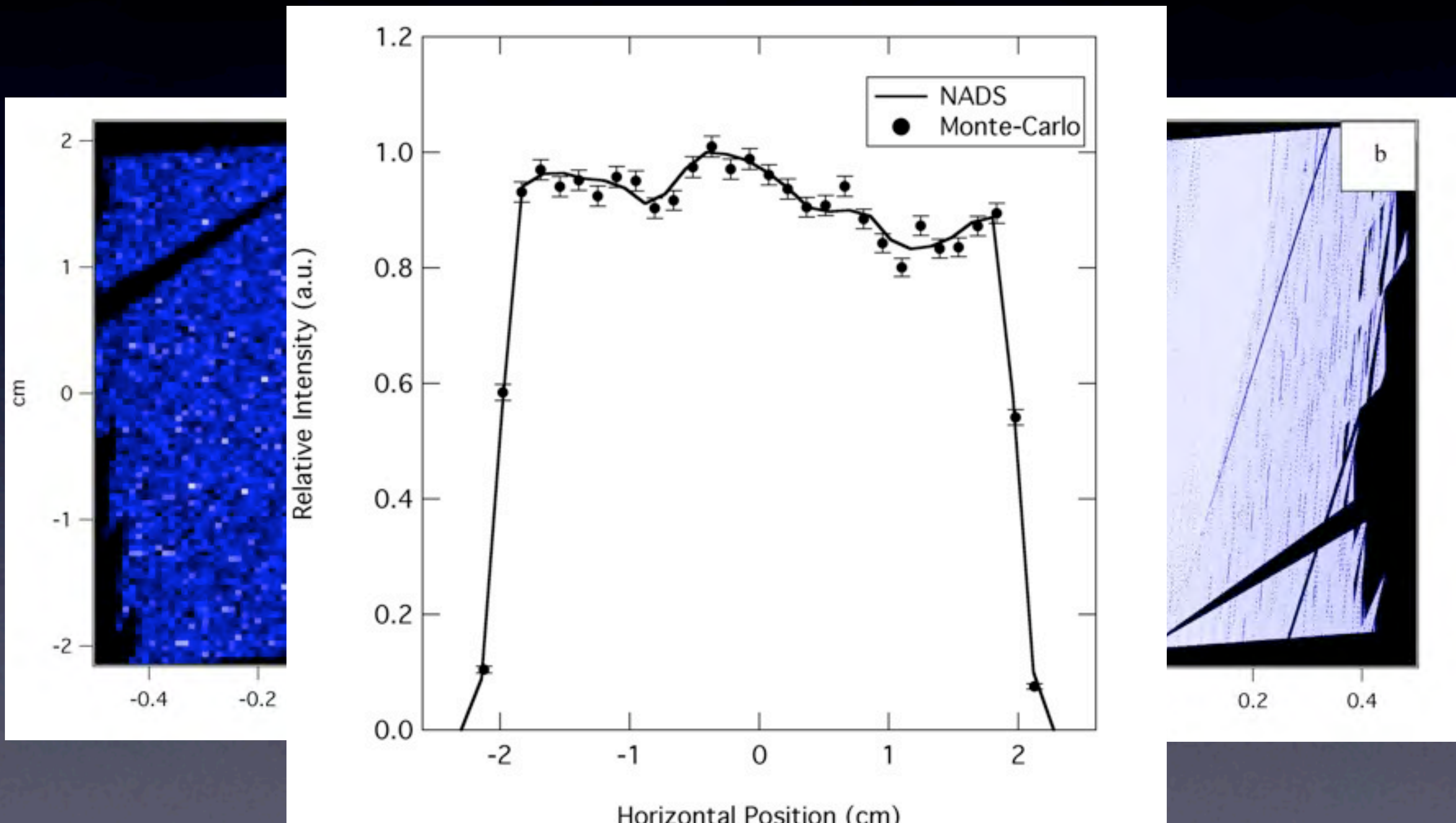
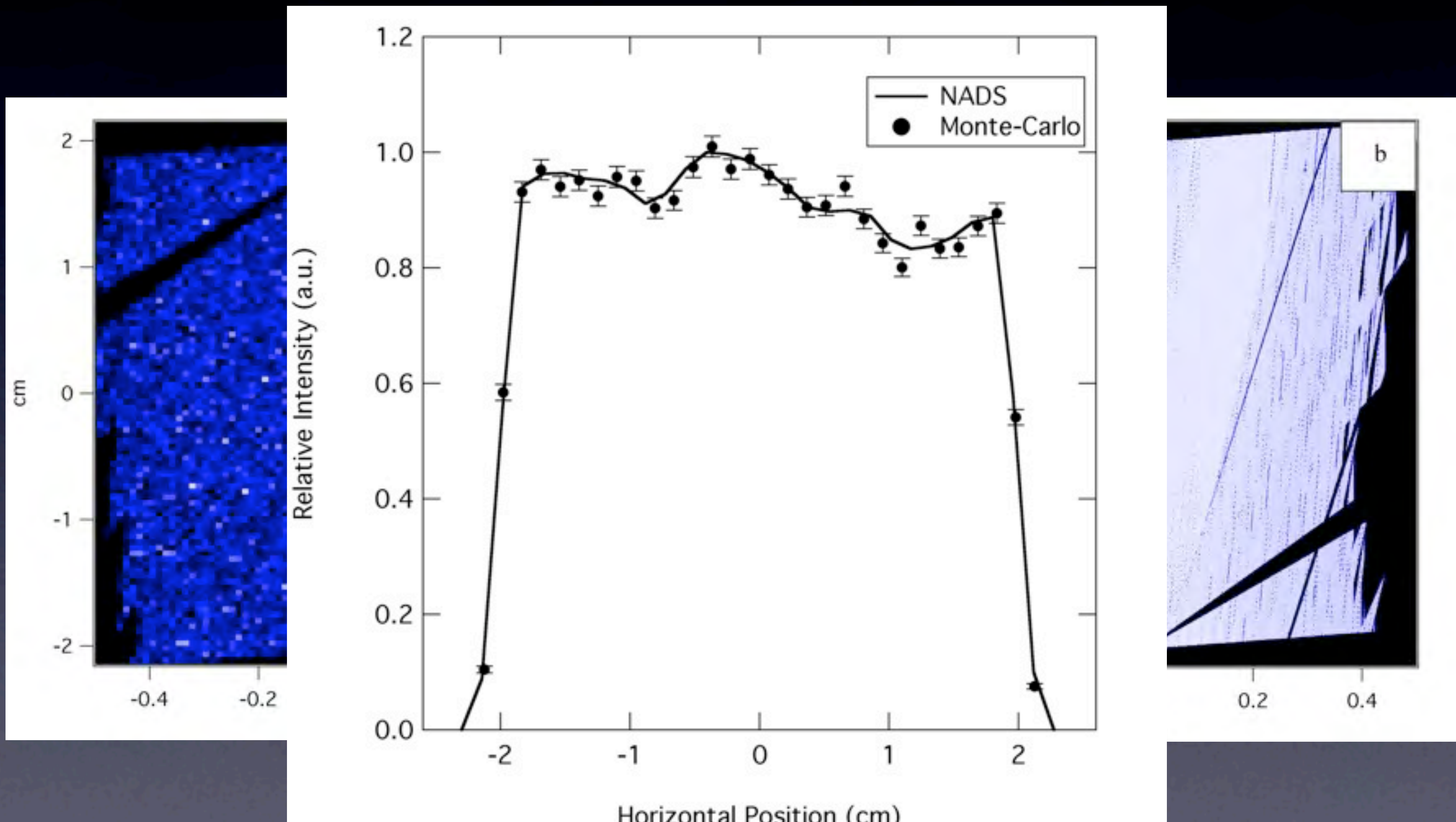


NADS
Monte-Carlo
Relative Intensity (a.u.)
Horizontal Position (cm)
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-2
-1
0
1
2
cm
-0.4
-0.2
0.2
0.4
b

Test 2: D22 (H)



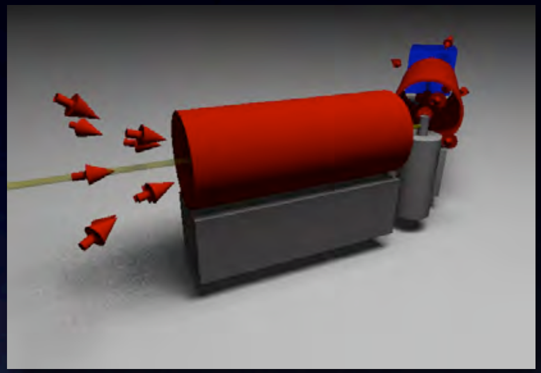
Calculate flux on sample: 55 ms

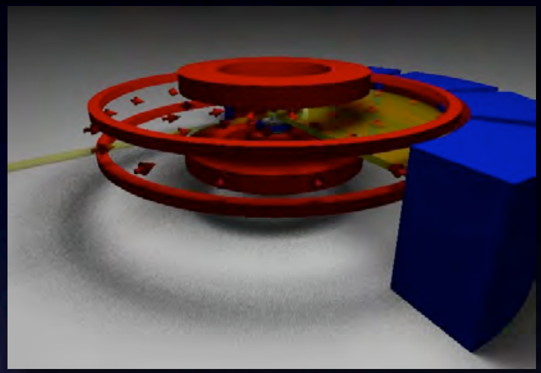
Test 3: WASP

- Agreement between NADS and MCSTAS *on sample*

- MCSTAS model Independently calculated by Peter Fouquet from moderator to Sample

- ~5 seconds for nads per wavelength (3 mins for white beam)





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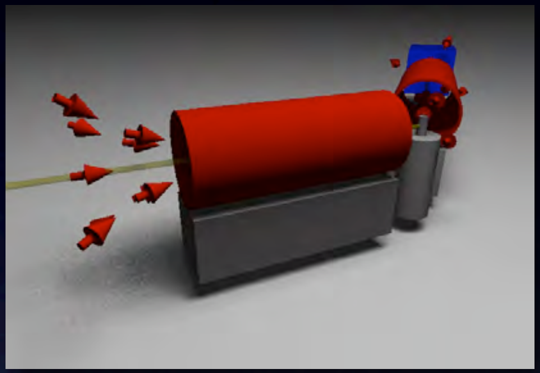
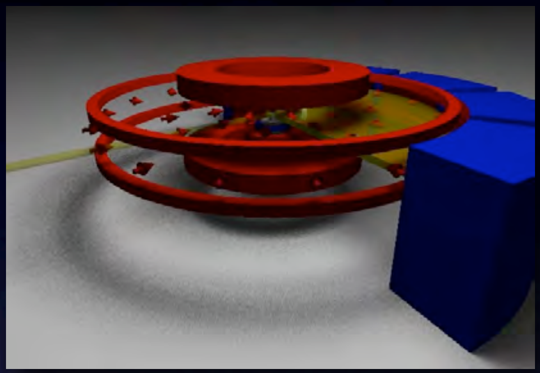
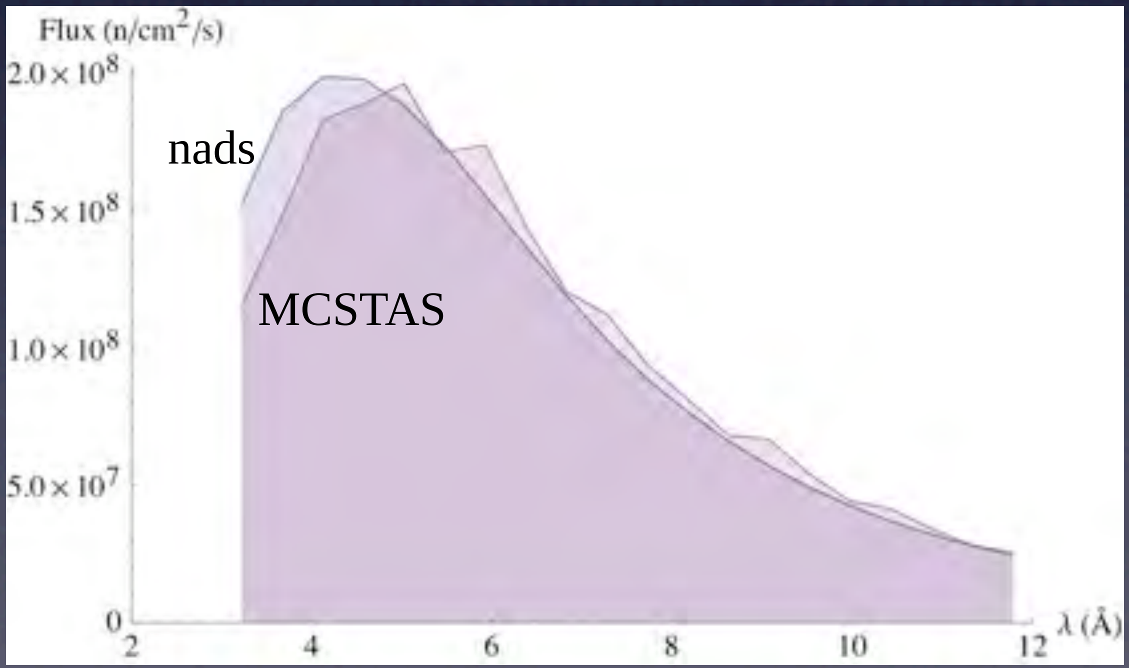
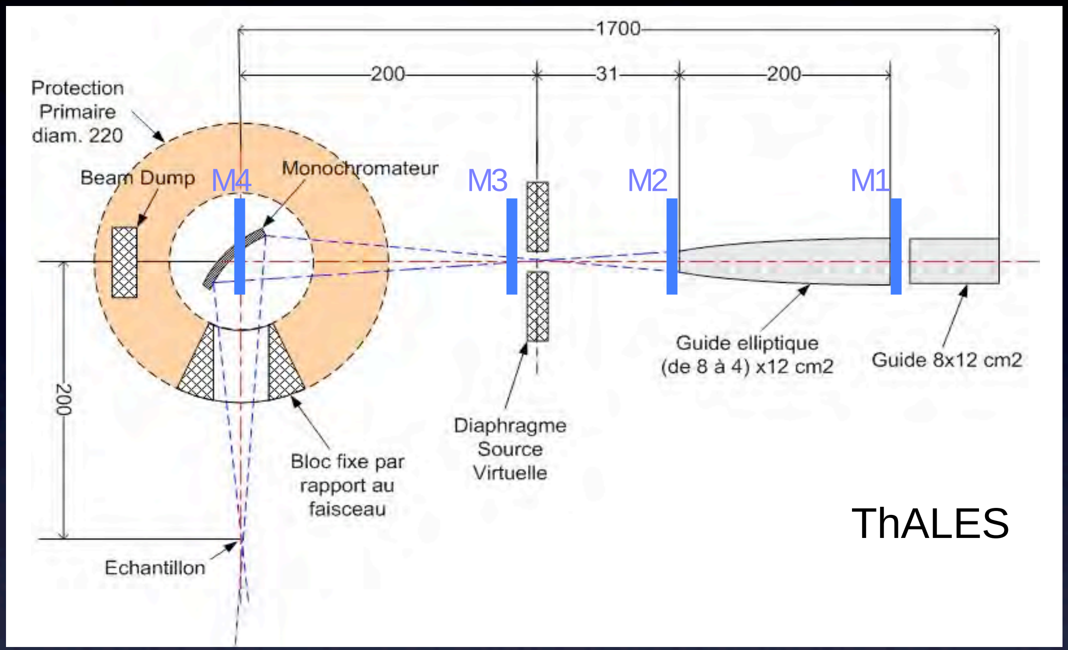






Test 4: Thales

- Agreement between SIMRES / RESTRAX and nads
- Trace up to virtual source (M3)
- ~40 ms for nads per wavelength (1.7 sec for white beam)



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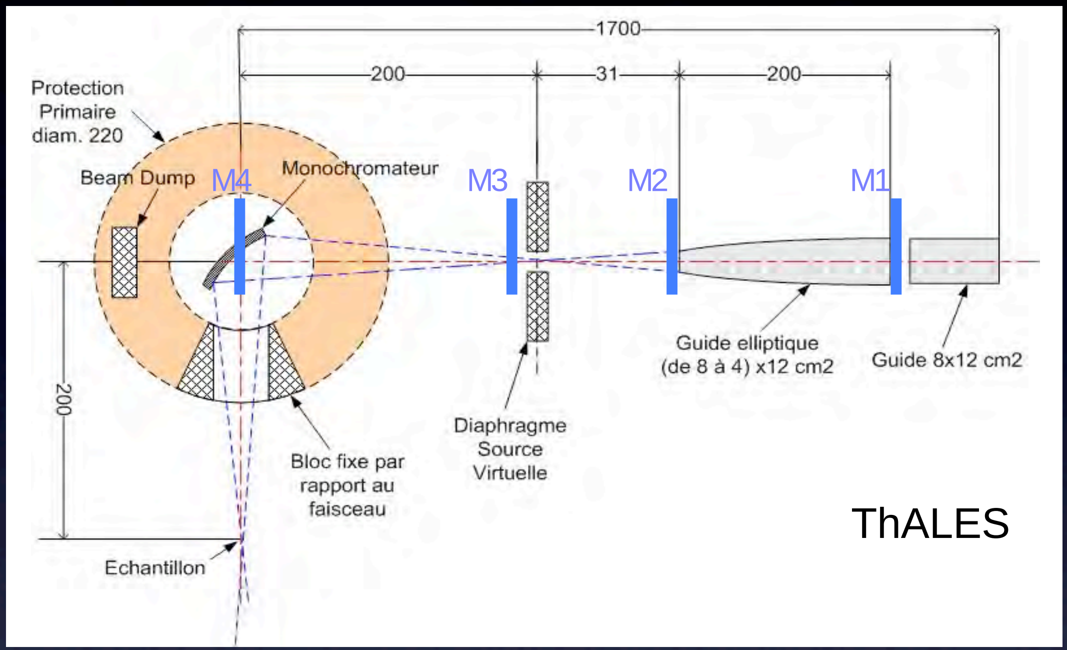

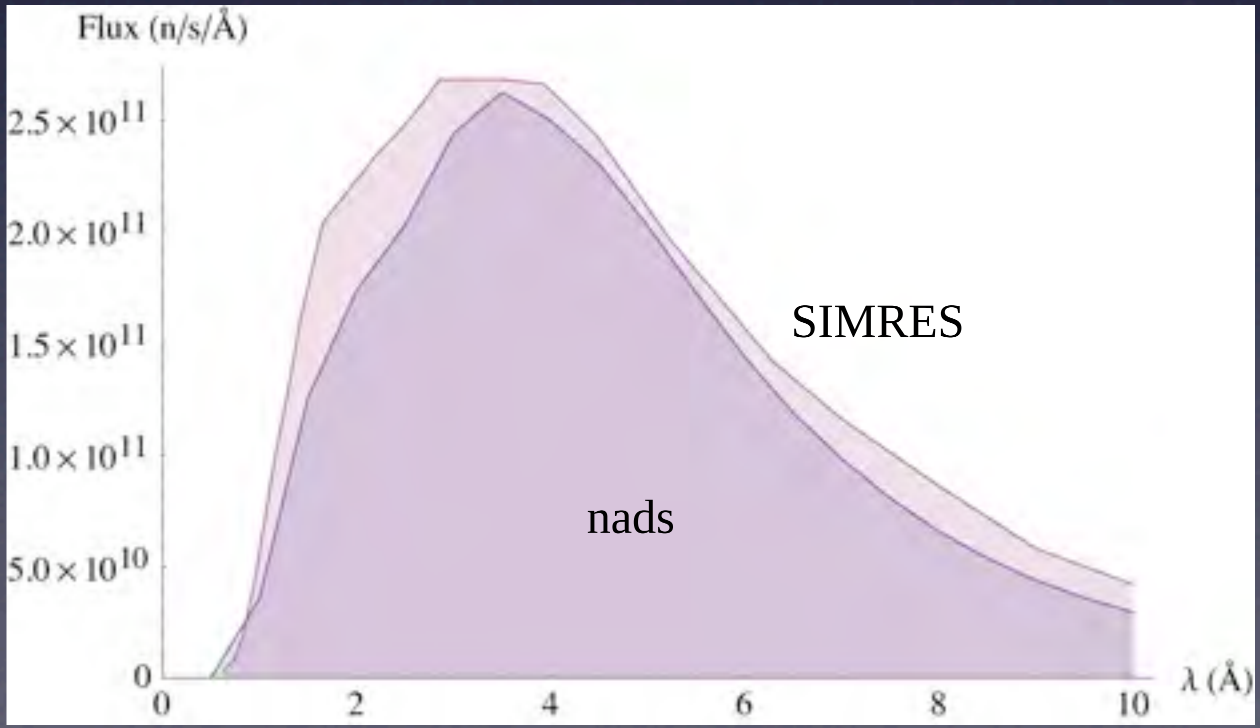

For Coders

- nads kernel in C++
- Understands xml input from file or pipe
- xml schema lets you check syntax of hand-coded simulations
- Uses getopt with varying degrees of verbosity
- nads -q prints only the output flux
- Fully scriptable using bash / c / mathematica...

```xml
<module>
    <rotation>
        <elemname>New Rotation Module</elemname>
        <hRotationAngle>0.6</hRotationAngle>
        <vRotationAngle>0</vRotationAngle>
    </rotation>
</module>
<module>
    <convergingGuide>
        <elemname>Separator</elemname>
        <width>8</width>
        <height>12</height>
        <exitWidth>18</exitWidth>
        <exitHeight>12</exitHeight>
        <length>2.77</length>
        <mnumber>3</mnumber>
    </convergingGuide>
</module>
```

Live Demonstration

- GUI
- 3d instrument visualisation with OpenGL
- Mathematica scripts

Limitations

- Each nads calculation is monochromatic (white beam possible via looping)
- Small angle approximation
- Separable vertical & horizontal channels
- Round objects approximated by rectangular objects of equal area (round sources etc)

Acknowledgements

- **ESFRI**
- **Ken Andersen**
- Klaus Habicht (HMI / BLZ)
- Leo Cussen (Cussen Consulting)